

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_M\DATA\BM013018\
 Data File : BM014013.D
 Acq On : 31 Jan 2018 00:35
 Operator : SJ/JU
 Sample : J1315-14
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 F6C71

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 1 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM011018.M
 Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.128	20	24	29	rBV3	33830	45573	1.27%	0.113%
2	6.751	634	640	657	rBV	469430	894340	24.84%	2.224%
3	6.910	661	667	677	rBV	370597	599421	16.65%	1.491%
4	7.098	692	699	712	rBV	557357	958577	26.62%	2.384%
5	7.563	772	778	789	rBV	416164	716535	19.90%	1.782%
6	8.281	893	900	915	rBV	622954	1142939	31.74%	2.842%
7	8.722	968	975	986	rBV	548214	970417	26.95%	2.413%
8	9.116	1037	1042	1047	rVB3	22103	37084	1.03%	0.092%
9	9.439	1084	1097	1109	rBV	447975	875800	24.32%	2.178%
10	9.975	1181	1188	1203	rBV	611427	1218934	33.85%	3.031%
11	10.339	1241	1250	1260	rBV	568038	962123	26.72%	2.393%
12	10.492	1267	1276	1295	rBV2	471079	1078509	29.95%	2.682%
13	13.639	1803	1811	1816	rBV	1287155	1851869	51.43%	4.605%
14	13.686	1816	1819	1833	rVB	253191	426596	11.85%	1.061%
15	13.910	1850	1857	1868	rBV	1444291	2185082	60.69%	5.434%
16	14.121	1888	1893	1898	rBV2	50250	76017	2.11%	0.189%
17	14.215	1902	1909	1919	rVV2	782403	1247744	34.65%	3.103%
18	14.462	1945	1951	1967	rBV2	241394	644599	17.90%	1.603%
19	14.751	1995	2000	2006	rVB7	19001	40270	1.12%	0.100%
20	15.080	2052	2056	2060	rBV2	75138	92952	2.58%	0.231%
21	15.221	2073	2080	2088	rBV	1730689	2609622	72.48%	6.490%
22	15.368	2099	2105	2118	rBV	348815	638055	17.72%	1.587%
23	15.462	2118	2121	2125	rBV3	29497	45025	1.25%	0.112%
24	15.598	2139	2144	2149	rBV3	41658	68576	1.90%	0.171%
25	15.945	2199	2203	2212	rVB3	58647	99718	2.77%	0.248%
26	16.356	2265	2273	2279	rBV2	90187	133487	3.71%	0.332%
27	16.433	2279	2286	2289	rBV5	34377	59337	1.65%	0.148%
28	16.974	2373	2378	2385	rVB2	1053282	1457959	40.49%	3.626%
29	17.074	2385	2395	2408	rBV2	1896135	2924174	81.21%	7.272%
30	17.209	2415	2418	2425	rVB8	26666	43584	1.21%	0.108%
31	17.756	2504	2511	2516	rBV3	87318	154089	4.28%	0.383%
32	17.880	2528	2532	2543	rVV2	271255	483800	13.44%	1.203%
33	18.156	2575	2579	2586	rBV6	23779	47851	1.33%	0.119%
34	18.721	2670	2675	2682	rBV	208435	274969	7.64%	0.684%

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35	18.786	2682	2686	2694	rVB3	73099	136345	3.79%	0.339%
36	19.015	2721	2725	2729	rBV3	80903	123664	3.43%	0.308%
37	19.168	2748	2751	2761	rBV4	110617	193972	5.39%	0.482%
38	19.268	2765	2768	2772	rVV4	66004	89066	2.47%	0.221%
39	19.380	2781	2787	2794	rVB	2416872	3341373	92.80%	8.310%
40	19.750	2845	2850	2853	rBV6	31353	52904	1.47%	0.132%
41	19.815	2856	2861	2864	rBV2	122605	165757	4.60%	0.412%
42	19.856	2865	2868	2873	rBV2	75646	94388	2.62%	0.235%
43	19.921	2875	2879	2882	rBV4	37834	55891	1.55%	0.139%
44	20.297	2940	2943	2945	rBV4	34195	37323	1.04%	0.093%
45	20.550	2982	2986	2990	rBV	323718	359960	10.00%	0.895%
46	20.615	2993	2997	3001	rVB	140131	170301	4.73%	0.424%
47	20.821	3030	3032	3035	rVB2	42537	37387	1.04%	0.093%
48	20.897	3041	3045	3058	rBV	401755	688416	19.12%	1.712%
49	20.997	3059	3062	3069	rBV4	100395	159416	4.43%	0.396%
50	21.056	3069	3072	3074	rBV3	59037	69817	1.94%	0.174%
51	21.180	3088	3093	3102	rBV	1372617	1898166	52.72%	4.720%
52	21.415	3130	3133	3137	rVB	166909	193306	5.37%	0.481%
53	21.491	3144	3146	3150	rVB3	129296	144603	4.02%	0.360%
54	22.068	3240	3244	3249	rBV	358944	453573	12.60%	1.128%
55	22.138	3253	3256	3261	rVB3	157301	195424	5.43%	0.486%
56	22.327	3285	3288	3293	rVB2	166050	220678	6.13%	0.549%
57	23.038	3406	3409	3414	rVB3	104079	154580	4.29%	0.384%
58	23.221	3434	3440	3450	rVB2	1897510	3600648	100.00%	8.954%
59	23.362	3458	3464	3473	rVB	927442	1824476	50.67%	4.537%
60	23.944	3558	3563	3573	rBV3	296534	644216	17.89%	1.602%

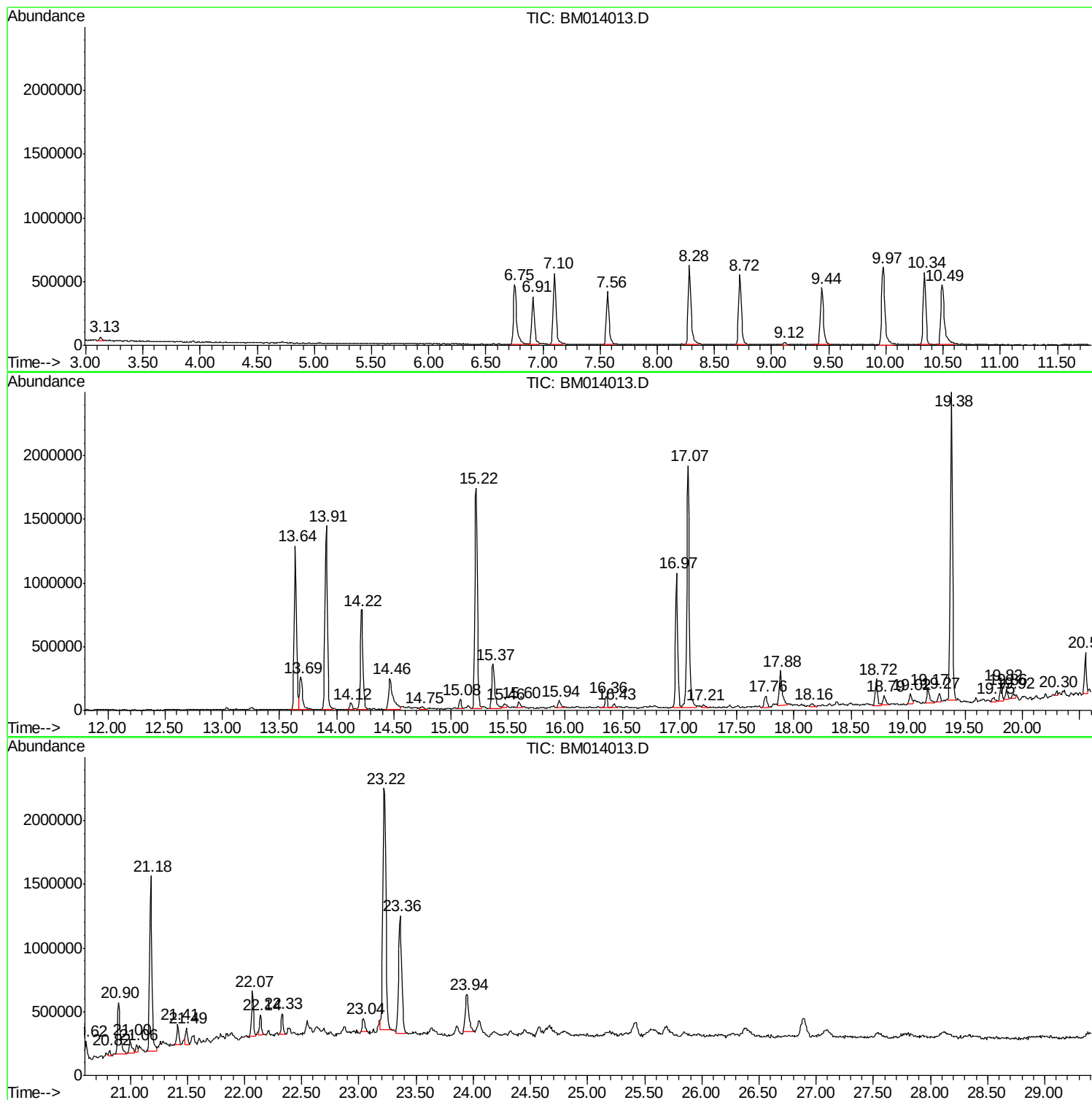
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TIC Library : C:\DATABASE\NIST11.L
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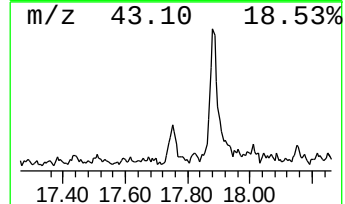
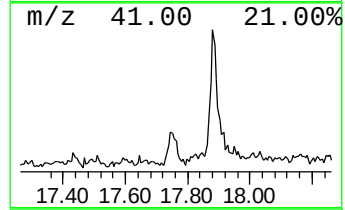
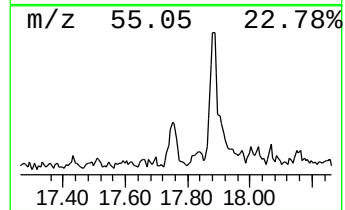
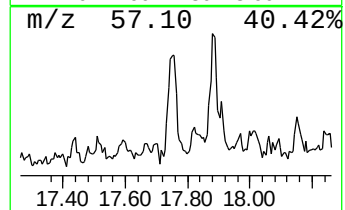
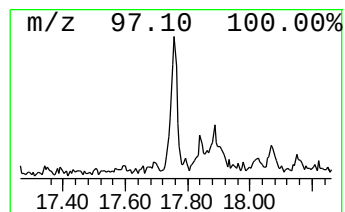
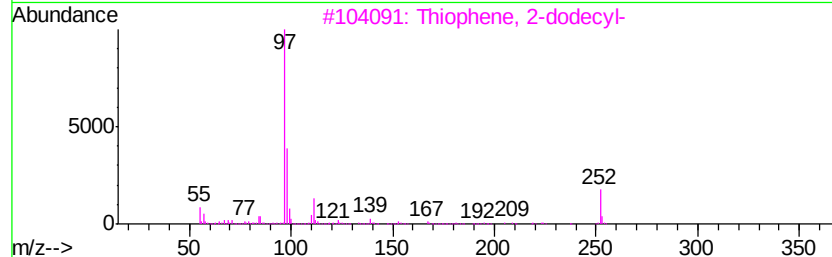
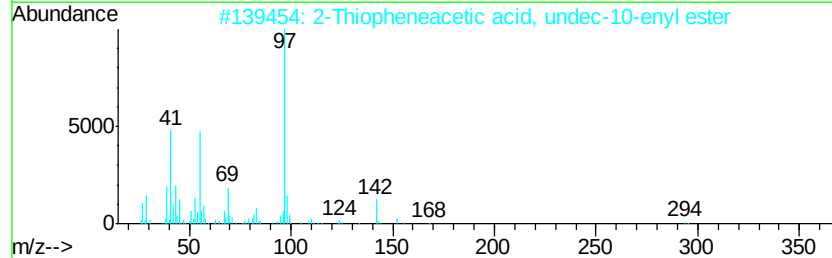
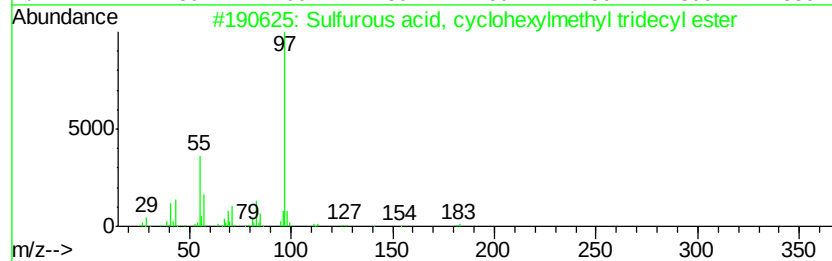
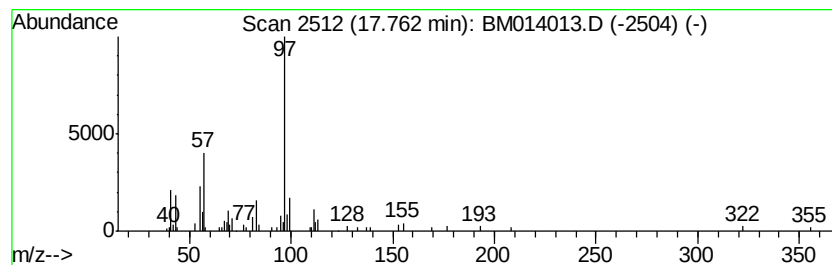
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM011018.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfurous acid, cyclohexylm... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.76	2.11 ng/ul	154089	Phenanthrene-d10	16.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, cyclohexylmethyl...	360	C20H40O3S	1000309-22-1	53
2		2-Thiopheneacetic acid, undec-10...	294	C17H26O2S	1000278-91-6	50
3		Thiophene, 2-dodecyl-	252	C16H28S	004861-61-4	45
4		Sulfurous acid, cyclohexylmethyl...	346	C19H38O3S	1000309-22-0	42
5		Oxalic acid, cyclohexylmethyl oc...	298	C17H30O4	1000309-68-4	40



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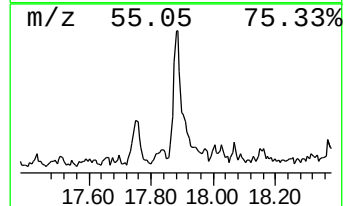
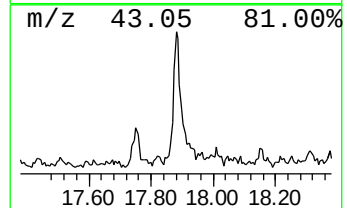
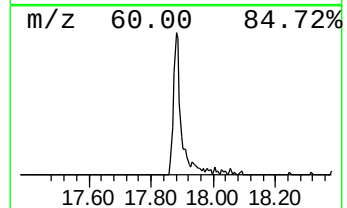
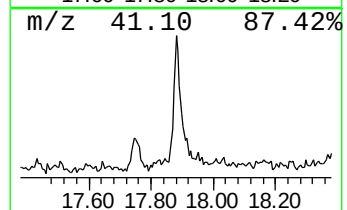
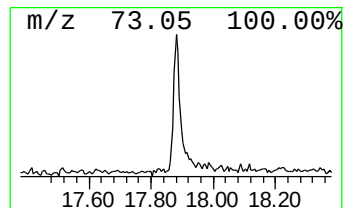
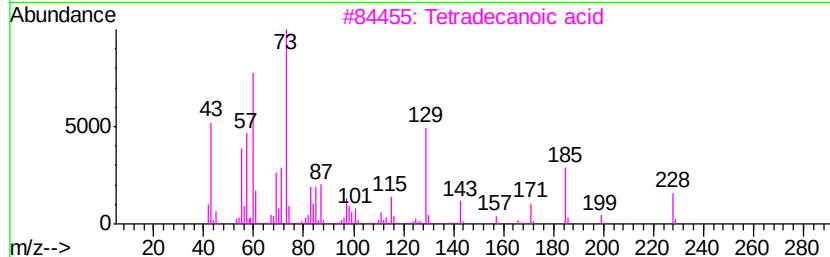
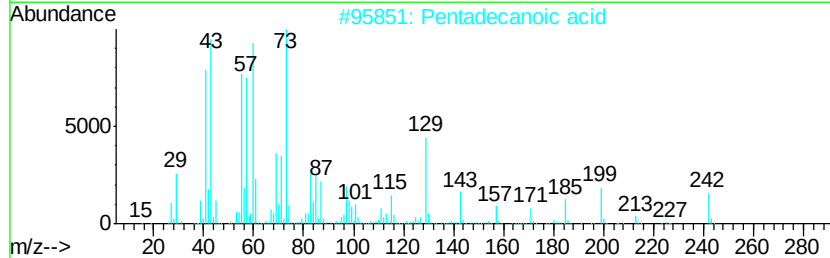
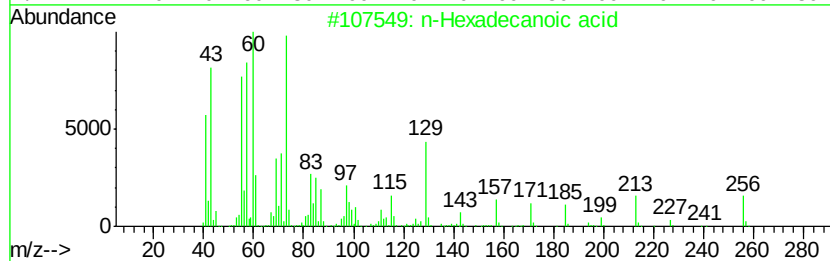
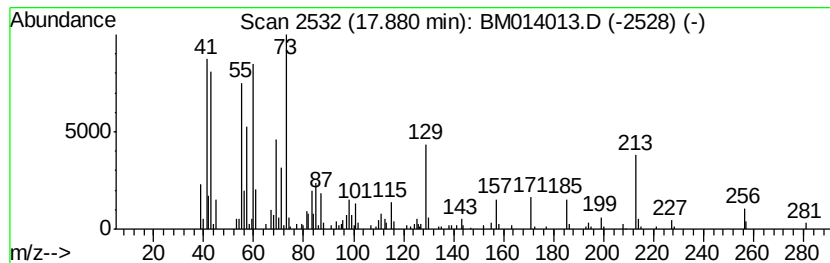
Instrument :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.88	6.64 ng/ul	483800	Phenanthrene-d10	16.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89	
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72	
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72	
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72	
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64	



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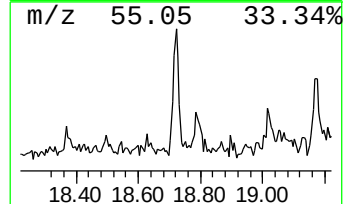
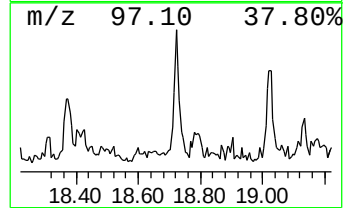
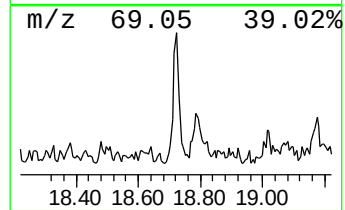
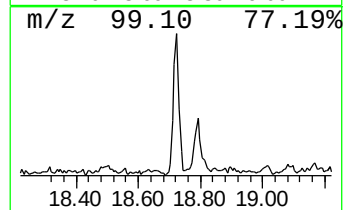
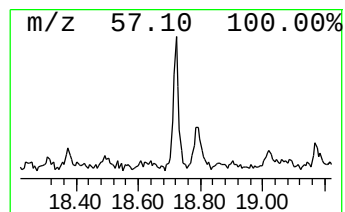
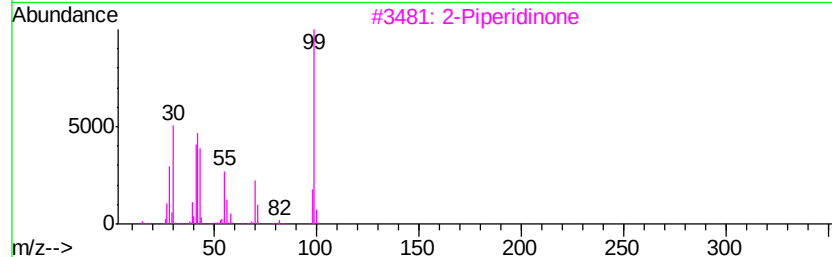
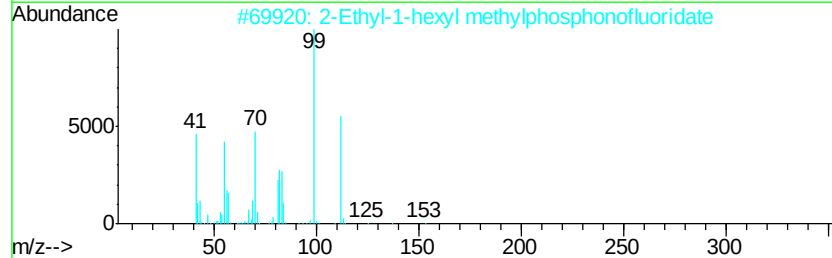
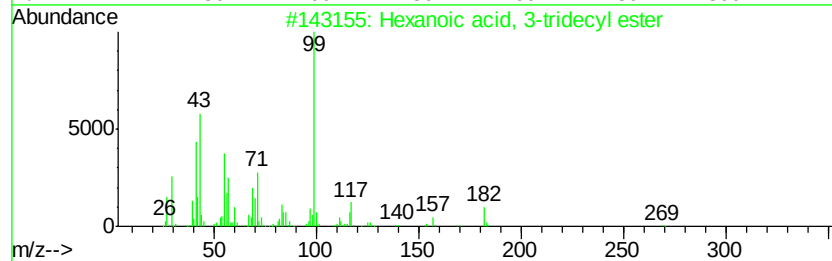
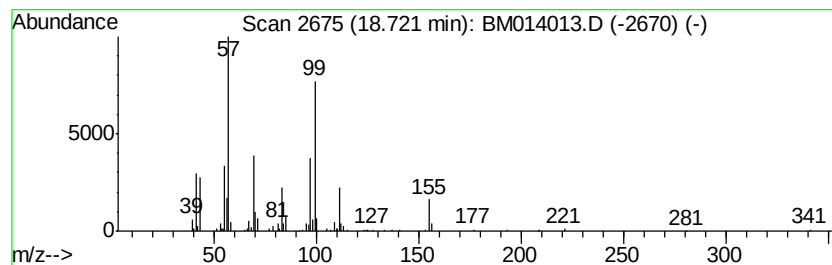
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Peak Number 3 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.72	3.77 ng/ul	274969	Phenanthrene-d10	16.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 3-tridecyl ester	298	C19H38O2	1000279-29-2	38
2		2-Ethyl-1-hexyl methylphosphonof...	210	C9H20F02P	000458-71-9	38
3		2-Piperidinone	99	C5H9NO	000675-20-7	38
4		Phosphonofluoridic acid, methyl-...	224	C10H22F02P	211192-74-4	38
5		Malonic acid, di(2,4-dimethylpen...	300	C17H32O4	1000349-02-5	37



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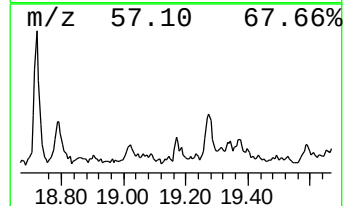
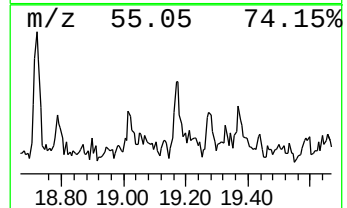
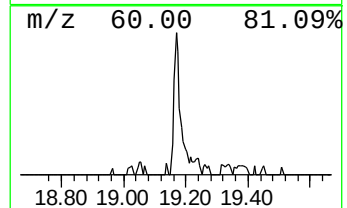
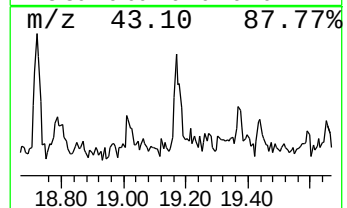
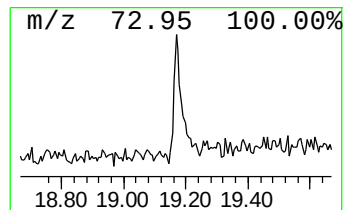
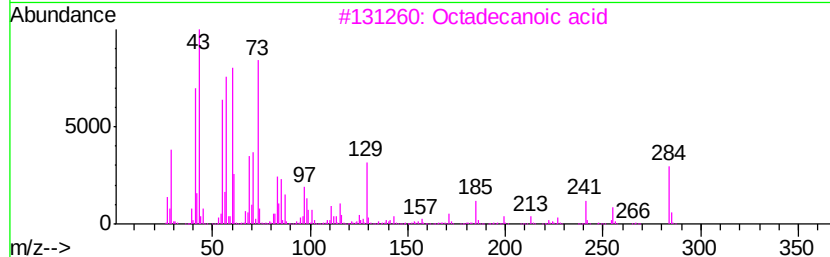
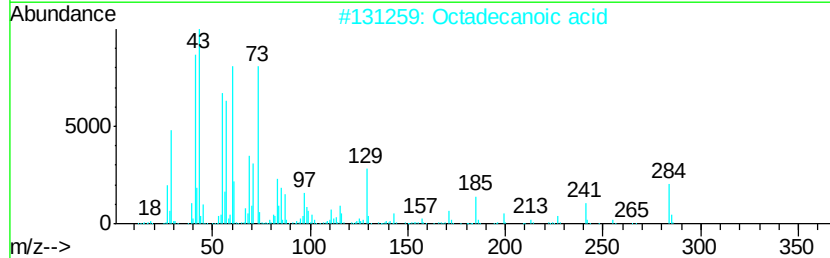
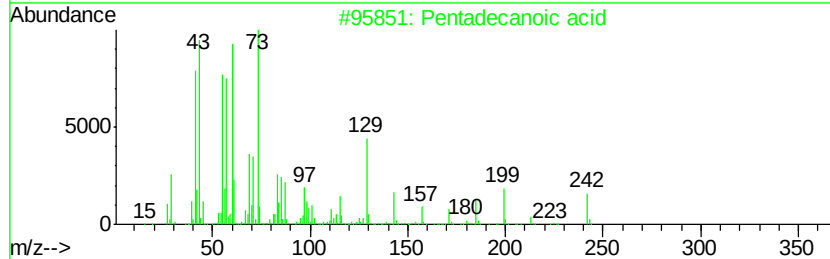
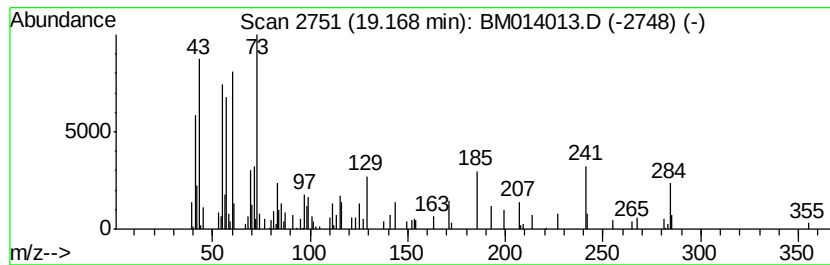
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.17	2.04 ng/ul	193972	Chrysene-d12	21.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2		Octadecanoic acid	284	C18H36O2	000057-11-4	76
3		Octadecanoic acid	284	C18H36O2	000057-11-4	70
4		Octadecanoic acid	284	C18H36O2	000057-11-4	62
5		n-Decanoic acid	172	C10H20O2	000334-48-5	55



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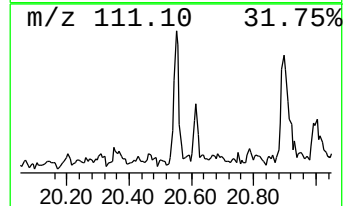
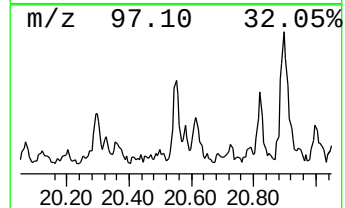
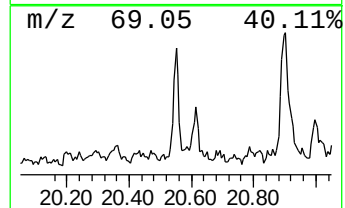
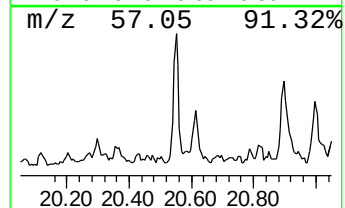
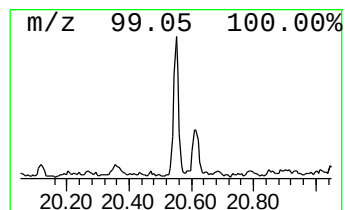
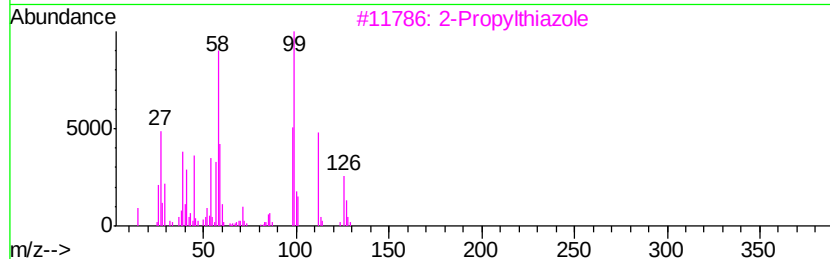
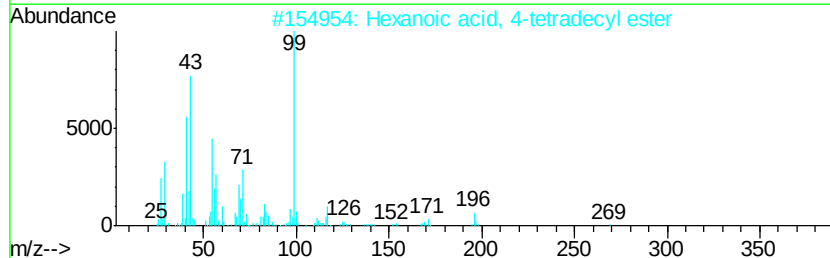
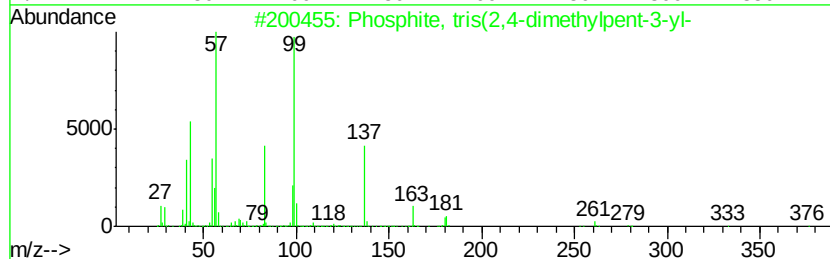
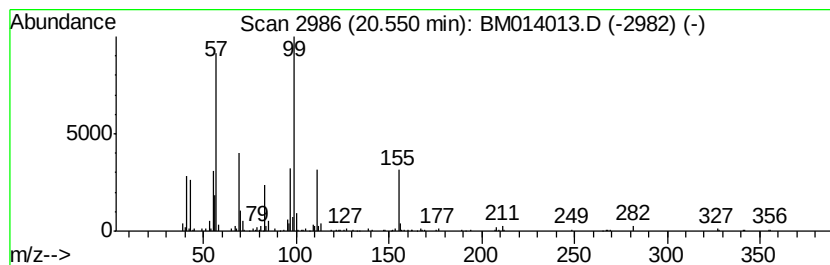
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.55	3.79 ng/ul	359960	Chrysene-d12	21.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phosphite, tris(2,4-dimethylpent...	376	C21H45O3P	1000159-84-4	43
2		Hexanoic acid, 4-tetradecyl ester	312	C20H40O2	1000279-29-8	38
3		2-Propylthiazole	127	C6H9NS	017626-75-4	38
4		Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	37
5		trans-3-Methyl-4-octanolide	156	C9H16O2	039638-67-0	37



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Acq On : 31 Jan 2018 00:35
Operator : SJ/JU
Sample : J1315-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

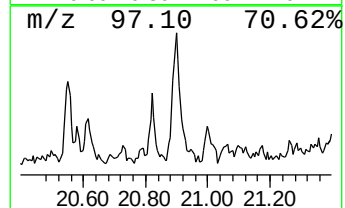
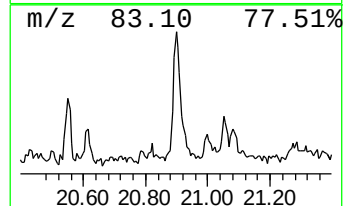
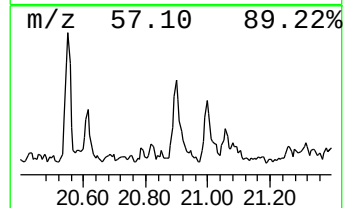
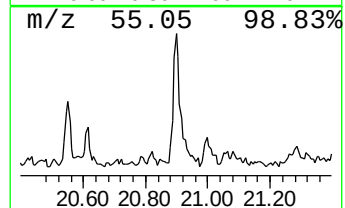
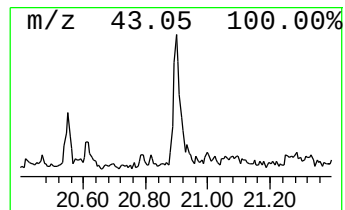
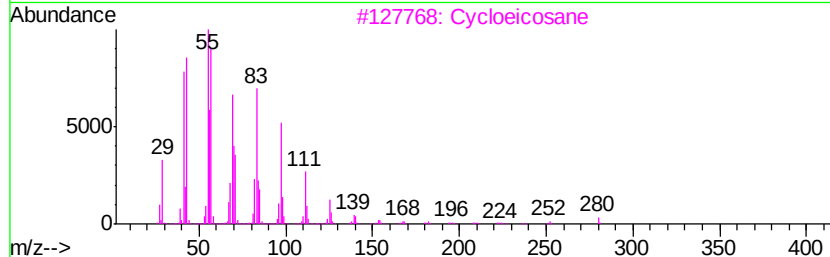
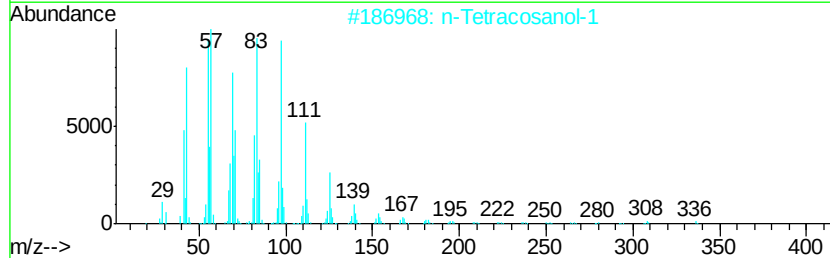
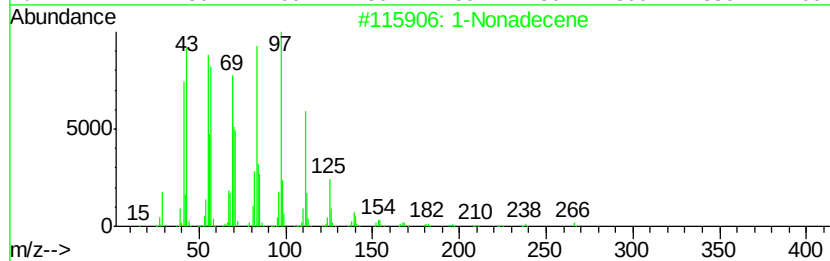
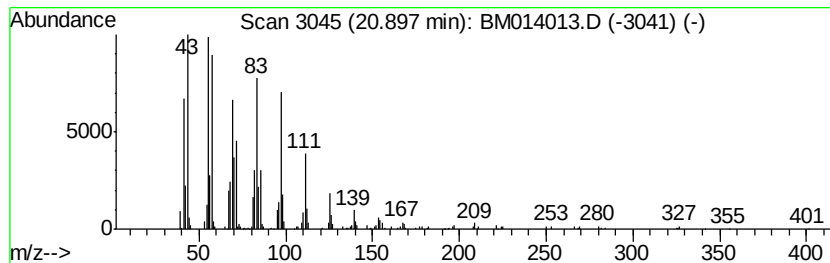
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 (DEL) Alkane: Cyclic20.90 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.90	7.25 ng/ul	688416	Chrysene-d12	21.18	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	98
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Cycloeicosane	280	C20H40	000296-56-0	94
4	1-Docosene	308	C22H44	001599-67-3	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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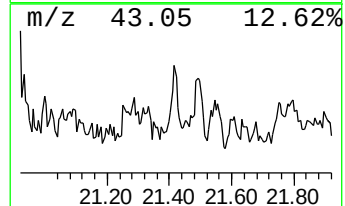
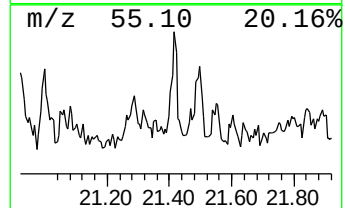
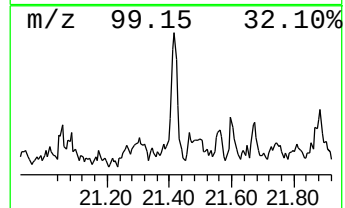
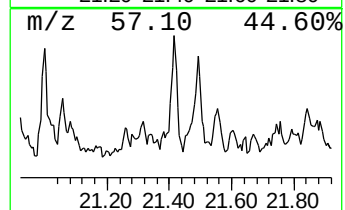
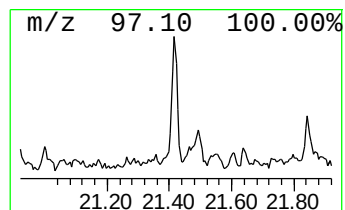
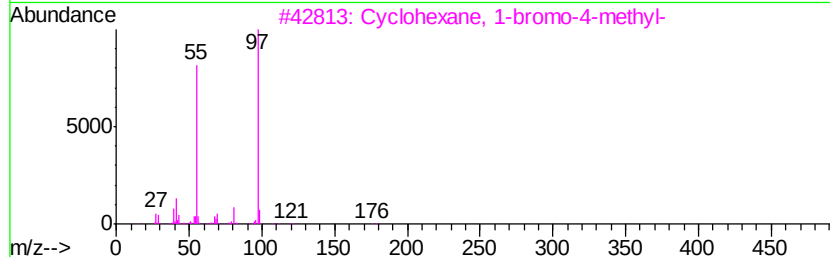
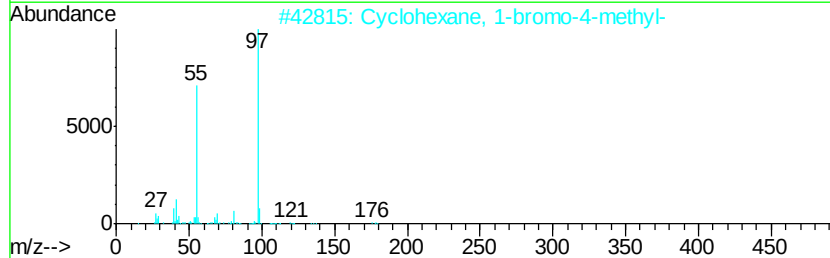
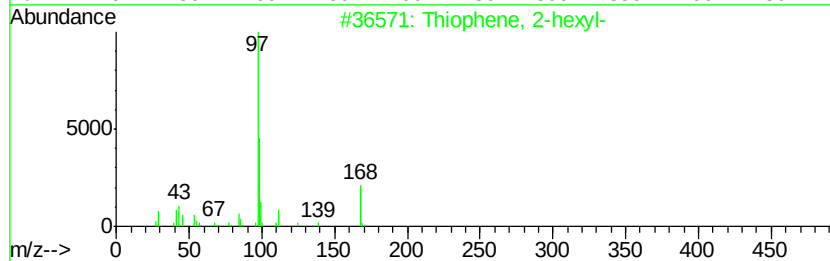
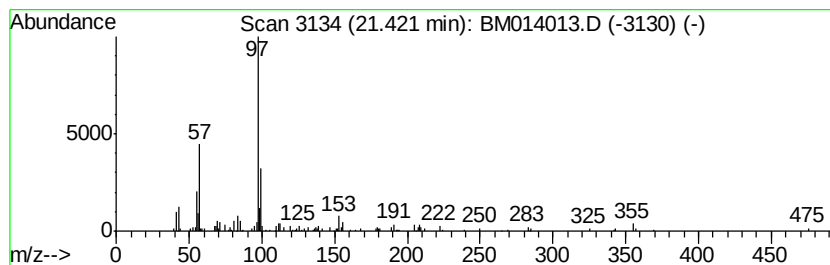
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Thiophene, 2-hexyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	2.04 ng/ul	193306	Chrysene-d12	21.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene, 2-hexyl-	168	C10H16S	018794-77-9	53
2		Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	53
3		Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	53
4		Oxazole, 2,4-dimethyl-	97	C5H7NO	007208-05-1	53
5		Cyclohexane, 1-bromo-3-methyl-	176	C7H13Br	013905-48-1	53



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_M\DATA\BM013018\
Data File : BM014013.D
Acq On : 31 Jan 2018 00:35
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Sample : J1315-14
Misc :
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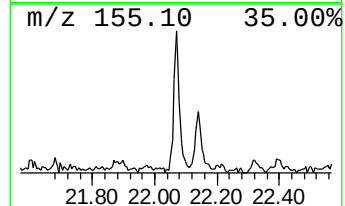
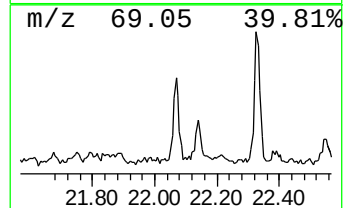
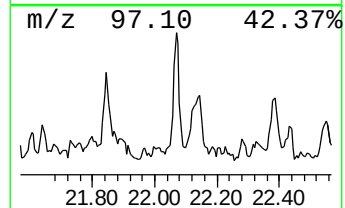
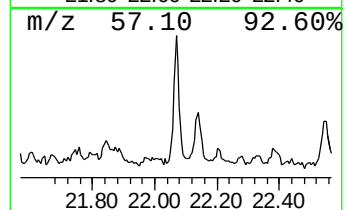
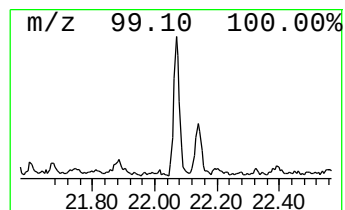
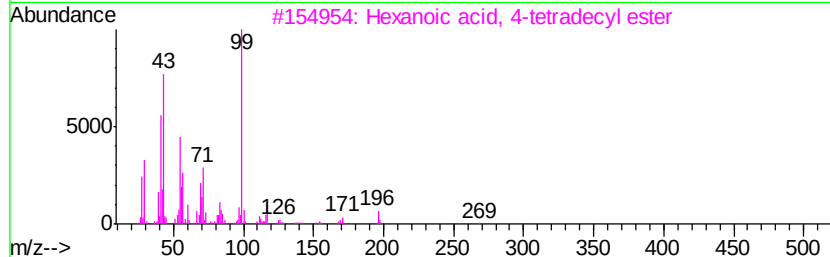
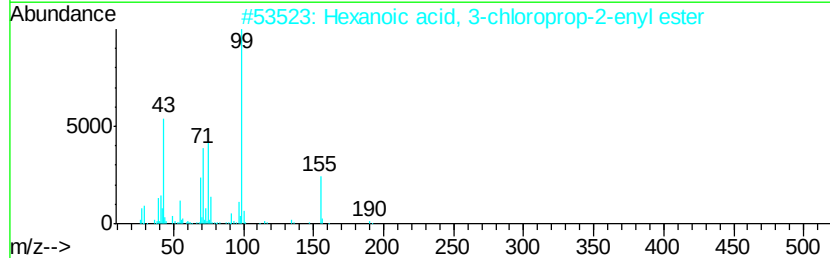
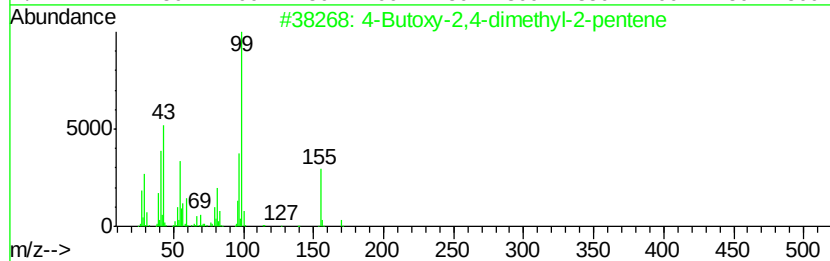
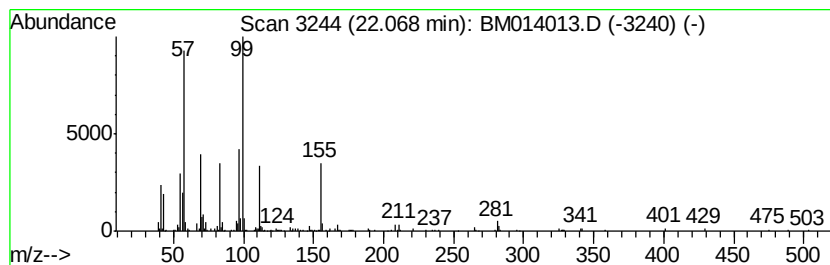
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 4-Butoxy-2,4-dimethyl-2-pen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	4.78 ng/ul	453573	Chrysene-d12	21.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	53
2		Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	43
3		Hexanoic acid, 4-tetradecyl ester	312	C20H40O2	1000279-29-8	35
4		4,6-Dimethyl-4-hydroxyhept-5-eno...	154	C9H14O2	1000122-47-0	35
5		Phosphite, tris(2,4-dimethylpent...	376	C21H45O3P	1000159-84-4	32



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_M\DATA\BM013018\
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Acq On : 31 Jan 2018 00:35
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Misc :
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Instrument :
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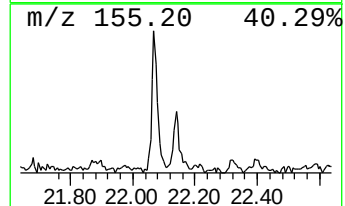
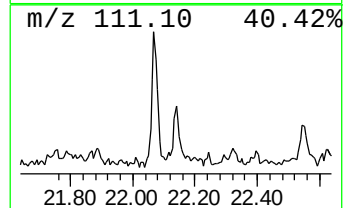
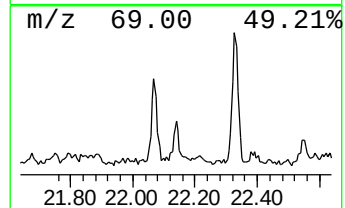
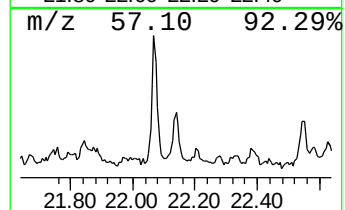
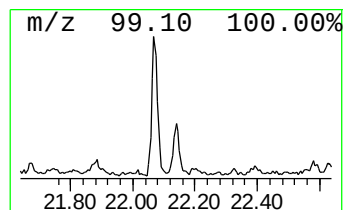
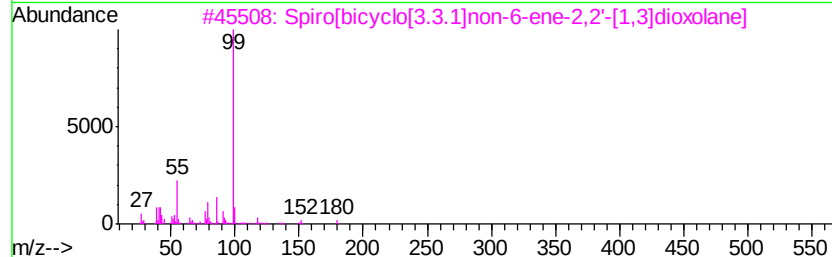
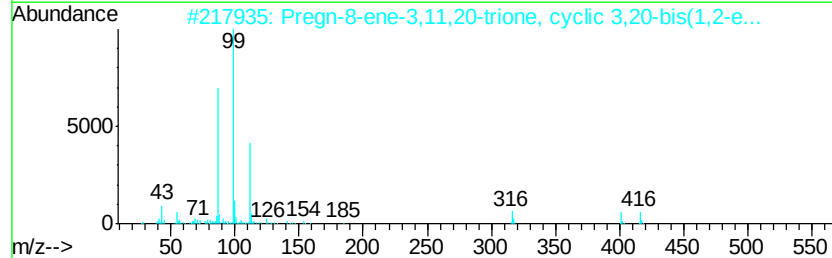
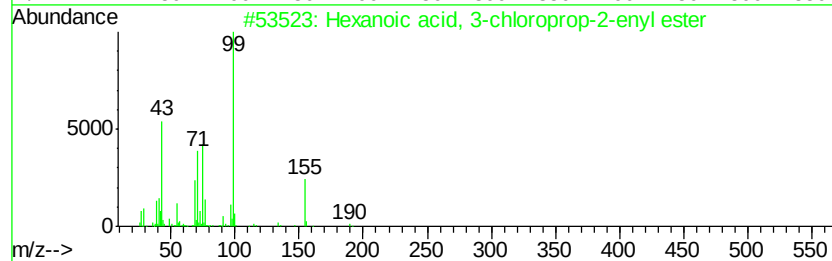
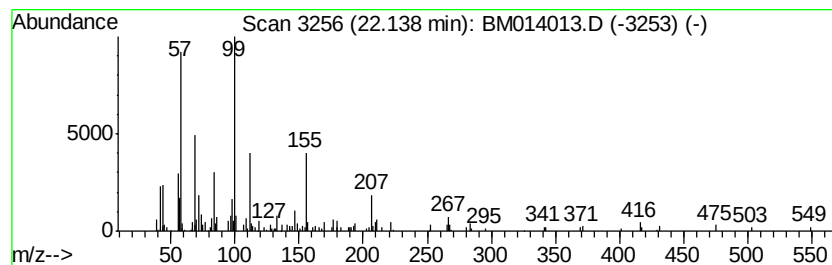
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Hexanoic acid, 3-chloroprop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.14	2.06 ng/ul	195424	Chrysene-d12	21.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	50
2		Pregn-8-ene-3,11,20-trione, cycl...	416	C25H36O5	021063-94-5	38
3		Spiro[bicyclo[3.3.1]non-6-ene-2,...	180	C11H16O2	029927-78-4	35
4		Benzoic acid, 4-[[2-(1-piperazin...	277	C14H19N3O3	1000350-32-6	35
5		Piperazine, 1-[2-(2,5-dimethyl-1...	207	C12H21N3	1000318-92-7	35



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_M\DATA\BM013018\
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Misc :
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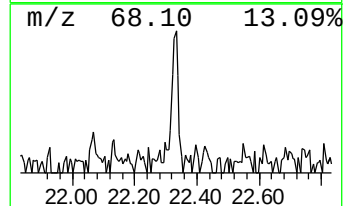
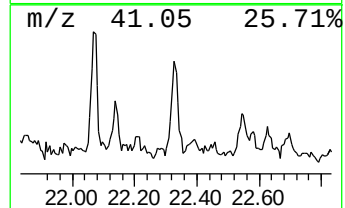
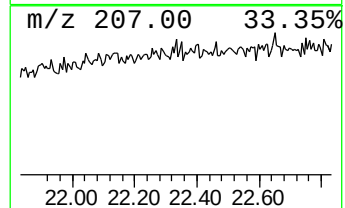
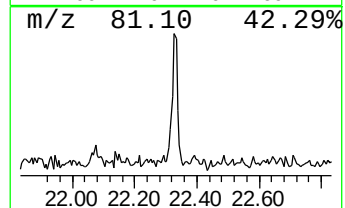
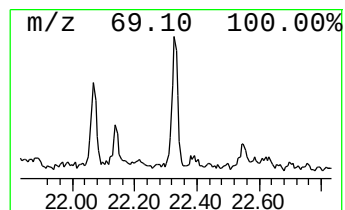
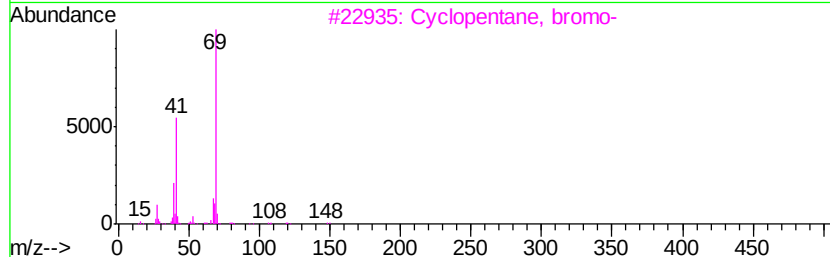
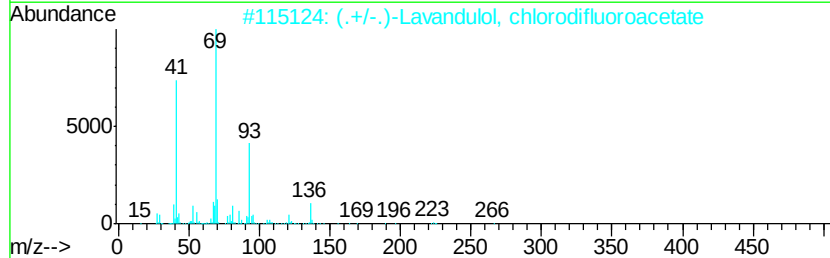
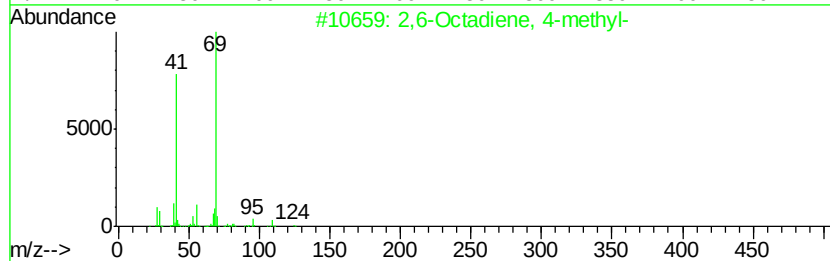
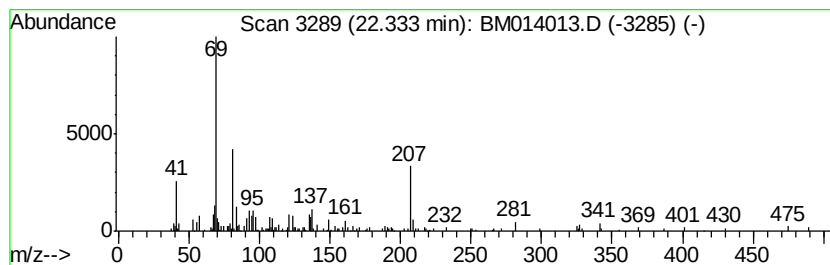
Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 2,6-Octadiene, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.33	2.42 ng/ul	220678	Perylene-d12	23.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2,6-Octadiene, 4-methyl-	124 C9H16	074498-94-5	64
2	(.+/-)-Lavandulol, chlorodifluo...	266 C12H17ClF2O2	1000376-22-9	64
3	Cyclopentane, bromo-	148 C5H9Br	000137-43-9	59
4	1,5-Heptadiene, 3,4-dimethyl-	124 C9H16	1000061-77-9	59
5	Cyclopentanecarboxylic acid, eth...	140 C8H12O2	016523-06-1	59



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_M\DATA\BM013018\
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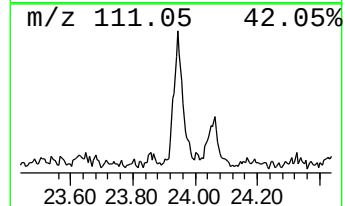
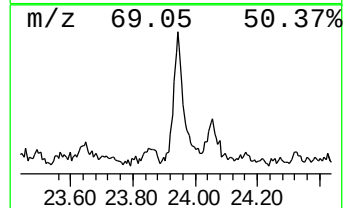
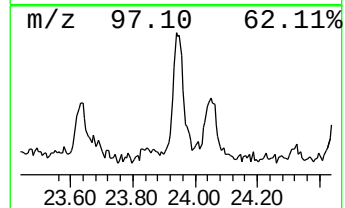
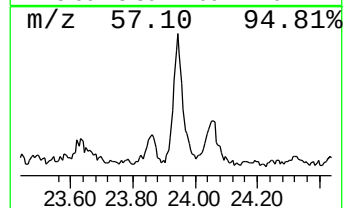
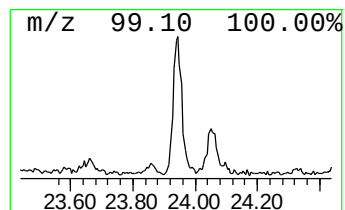
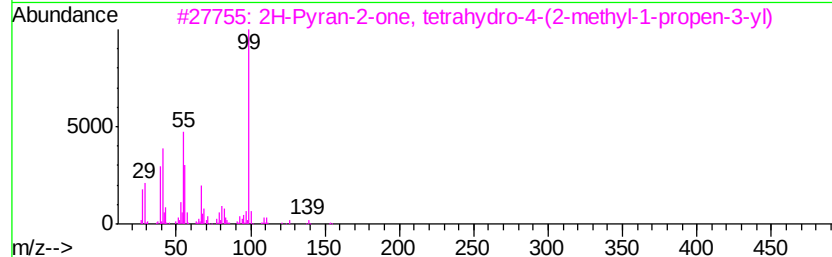
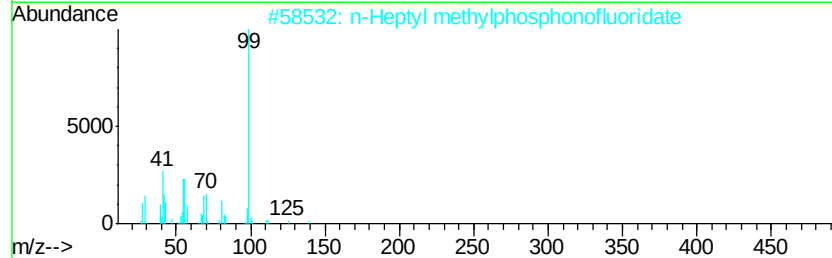
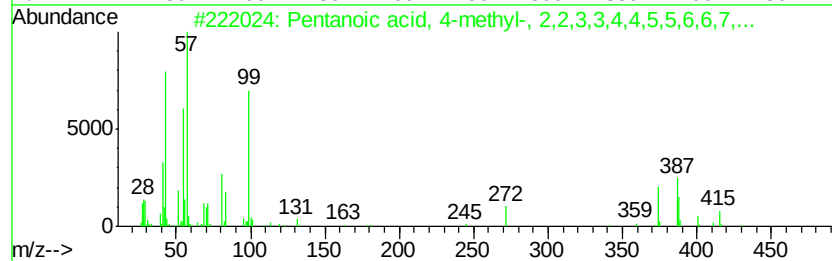
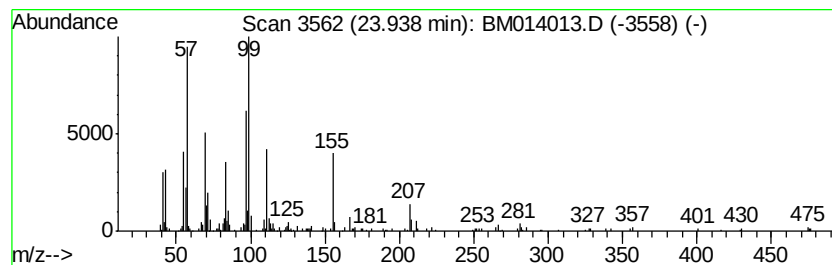
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.94	7.06 ng/ul	644216	Perylene-d12	23.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid, 4-methyl-, 2,2,3...	430	C13H14F12O2	1000141-64-1	27
2		n-Heptyl methylphosphonofluoridate	196	C8H18F02P	162085-82-7	22
3		2H-Pyran-2-one, tetrahydro-4-(2-...	154	C9H14O2	1000153-91-9	22
4		1,3-Cyclohexanedione, 5-isopropyl-	154	C9H14O2	018456-87-6	22
5		1,2-Dodecanediol	202	C12H26O2	001119-87-5	22



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_M\DATA\BM013018\
Data File : BM014013.D
Acq On : 31 Jan 2018 00:35
Operator : SJ/JU
Sample : J1315-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
F6C71

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM011018.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfurous acid, c...	17.76	2.1	ng/ul	154089	4	16.97	1457960	20.0
n-Hexadecanoic acid	17.88	6.6	ng/ul	483800	4	16.97	1457960	20.0
unknown-01	18.72	3.8	ng/ul	274969	4	16.97	1457960	20.0
Pentadecanoic acid	19.17	2.0	ng/ul	193972	5	21.18	1898170	20.0
unknown-02	20.55	3.8	ng/ul	359960	5	21.18	1898170	20.0
(DEL) Alkane: Cyc...	20.90	7.3	ng/ul	688416	5	21.18	1898170	20.0
Thiophene, 2-hexyl-	21.42	2.0	ng/ul	193306	5	21.18	1898170	20.0
4-Butoxy-2,4-dime...	22.07	4.8	ng/ul	453573	5	21.18	1898170	20.0
Hexanoic acid, 3-...	22.14	2.1	ng/ul	195424	5	21.18	1898170	20.0
2,6-Octadiene, 4-...	22.33	2.4	ng/ul	220678	6	23.36	1824480	20.0
unknown-03	23.94	7.1	ng/ul	644216	6	23.36	1824480	20.0