

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
 Data File : BM010611.D
 Acq On : 21 Jun 2017 03:54
 Operator : SJ/MA
 Sample : I3790-12
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C0B84

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-BM062017.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	6.646	635	639	645	rVB	79525	119700	2.39%	0.309%
2	6.816	661	668	676	rBV	256757	373763	7.48%	0.966%
3	7.004	693	700	708	rVB	301889	451786	9.04%	1.167%
4	7.463	773	778	785	rBV	296294	455175	9.11%	1.176%
5	8.169	892	898	907	rVB	255140	382483	7.65%	0.988%
6	8.610	967	973	980	rVB	367785	562730	11.26%	1.454%
7	9.322	1087	1094	1101	rBV2	340104	532211	10.65%	1.375%
8	9.587	1128	1139	1147	rBV3	61251	117473	2.35%	0.304%
9	9.851	1178	1184	1192	rVB	504021	794927	15.90%	2.054%
10	10.228	1241	1248	1255	rBV	423829	690402	13.81%	1.784%
11	10.739	1330	1335	1342	rBV	63547	88306	1.77%	0.228%
12	12.398	1612	1617	1624	rBV3	47869	74122	1.48%	0.192%
13	13.539	1805	1811	1817	rBV	1129530	1483873	29.68%	3.834%
14	13.804	1849	1856	1863	rBV	1075869	1543077	30.87%	3.987%
15	14.116	1903	1909	1920	rVB2	680261	1042146	20.85%	2.693%
16	14.322	1940	1944	1951	rVB	105783	144535	2.89%	0.373%
17	14.569	1980	1986	1995	rBV2	73686	99684	1.99%	0.258%
18	15.121	2074	2080	2087	rVB	1391115	1994969	39.91%	5.155%
19	15.239	2094	2100	2107	rBV	520081	700677	14.02%	1.810%
20	15.716	2176	2181	2186	rBV	274773	324920	6.50%	0.840%
21	15.768	2186	2190	2198	rVB	558261	654433	13.09%	1.691%
22	16.616	2330	2334	2338	rBV	63727	75700	1.51%	0.196%
23	16.704	2342	2349	2358	rVB	421274	607516	12.15%	1.570%
24	16.868	2371	2377	2384	rVB	1004717	1390513	27.82%	3.593%
25	16.968	2388	2394	2402	rVV	1683462	2371581	47.44%	6.128%
26	17.198	2427	2433	2437	rBV	1885216	2310133	46.21%	5.969%
27	17.251	2437	2442	2452	rVB	4358647	4998854	100.00%	12.916%
28	17.533	2485	2490	2492	rVV	75327	85893	1.72%	0.222%
29	17.563	2492	2495	2501	rVB2	127279	148608	2.97%	0.384%
30	17.798	2530	2535	2543	rBV2	117218	162946	3.26%	0.421%
31	18.133	2585	2592	2598	rBV	98767	143197	2.86%	0.370%
32	18.515	2651	2657	2661	rBV	148855	197223	3.95%	0.510%
33	18.562	2661	2665	2670	rVB	410547	466512	9.33%	1.205%
34	19.092	2750	2755	2763	rBV	290930	406505	8.13%	1.050%

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35	19.280	2779	2787	2796	rBV	2205516	3056135	61.14%	7.896%
36	19.368	2796	2802	2807	rVB3	54127	85328	1.71%	0.220%
37	19.656	2846	2851	2854	rBV	191750	215880	4.32%	0.558%
38	19.698	2854	2858	2866	rVB	451162	499005	9.98%	1.289%
39	20.639	3014	3018	3021	rBV	143730	157862	3.16%	0.408%
40	20.674	3021	3024	3031	rVB	289374	318109	6.36%	0.822%
41	21.086	3089	3094	3099	rBV	1533853	1878421	37.58%	4.853%
42	21.509	3162	3166	3168	rBV	179837	205283	4.11%	0.530%
43	21.539	3168	3171	3177	rVB	383120	410300	8.21%	1.060%
44	22.097	3262	3266	3269	rBV3	93826	121904	2.44%	0.315%
45	22.133	3269	3272	3277	rVB7	53247	80370	1.61%	0.208%
46	22.397	3313	3317	3320	rBV2	184975	255965	5.12%	0.661%
47	22.433	3320	3323	3331	rVB	363486	461021	9.22%	1.191%
48	22.615	3351	3354	3361	rVB5	48711	64945	1.30%	0.168%
49	23.097	3429	3436	3443	rVV2	1565063	2767878	55.37%	7.152%
50	23.156	3443	3446	3450	rVB3	65082	96201	1.92%	0.249%
51	23.227	3452	3458	3467	rVB	883504	1607115	32.15%	4.152%
52	23.768	3545	3550	3557	rVB3	76982	141940	2.84%	0.367%
53	24.468	3665	3669	3677	rVB6	82067	159662	3.19%	0.413%
54	25.280	3804	3807	3814	rVB6	61086	123234	2.47%	0.318%

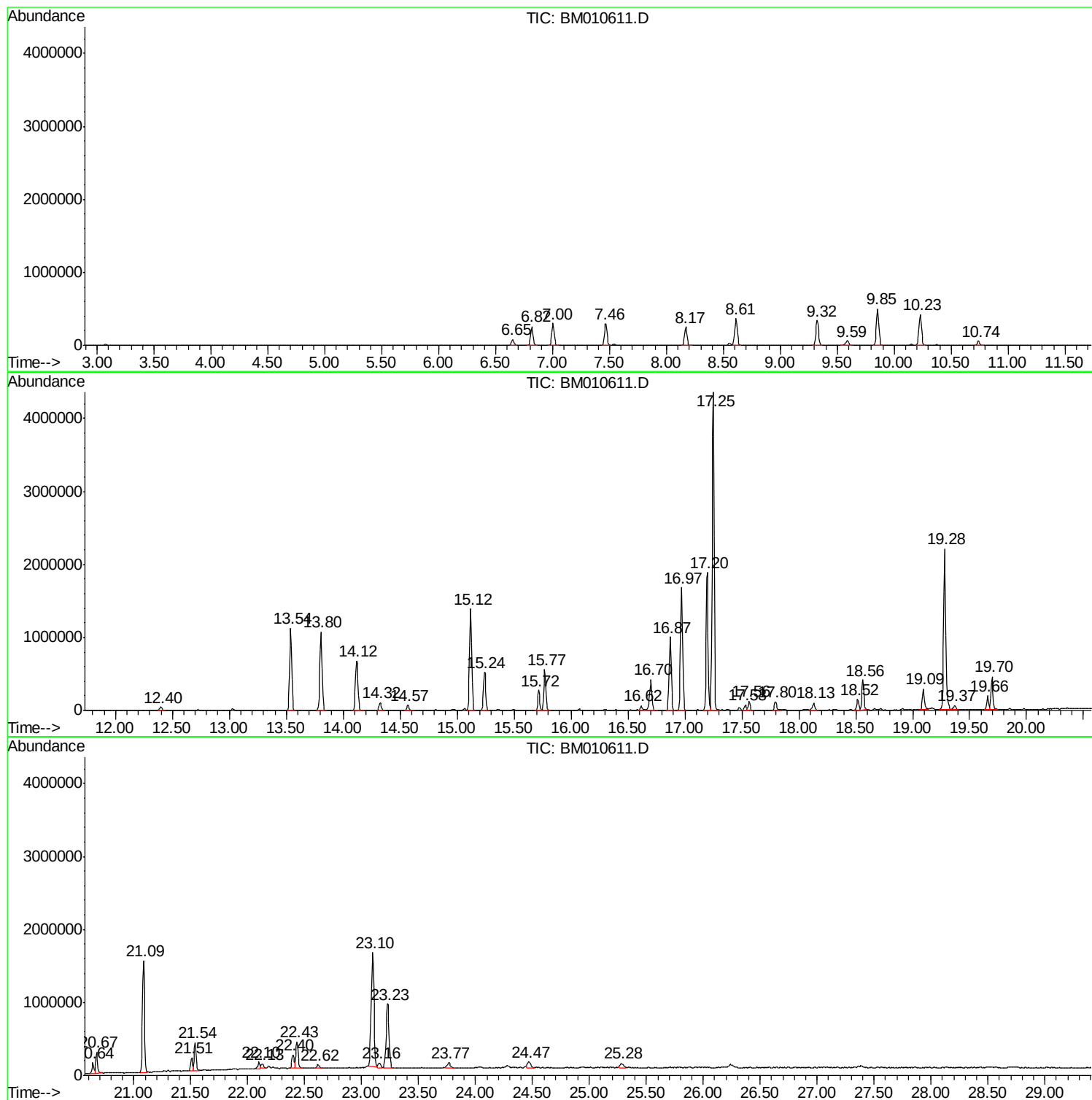
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Quant Title : SVOA CALIBRATION

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



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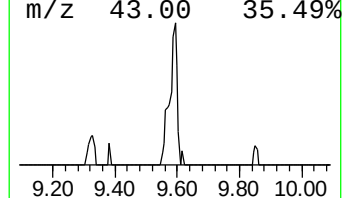
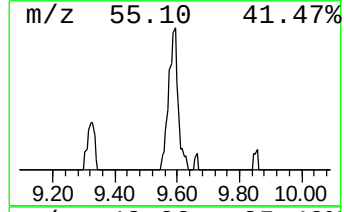
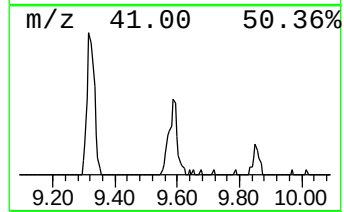
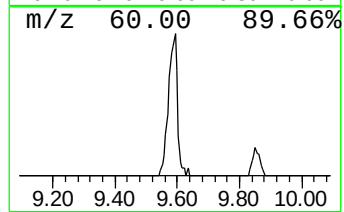
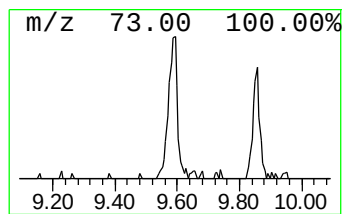
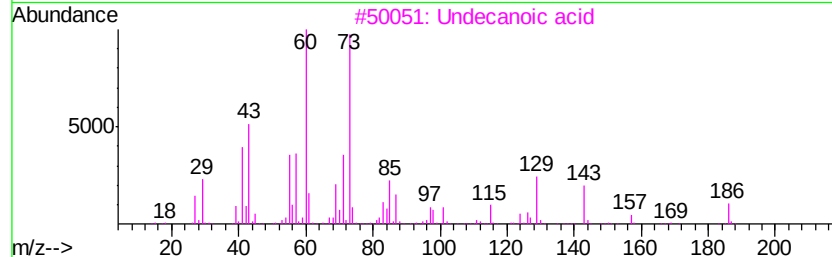
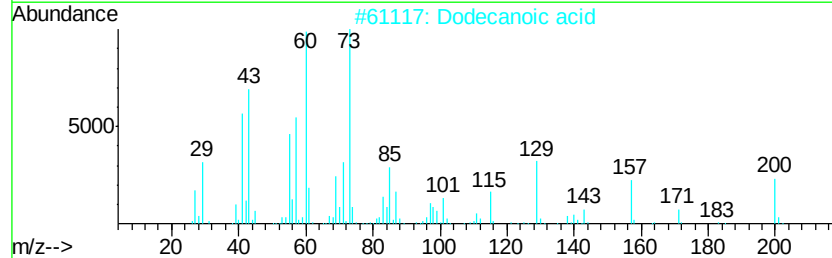
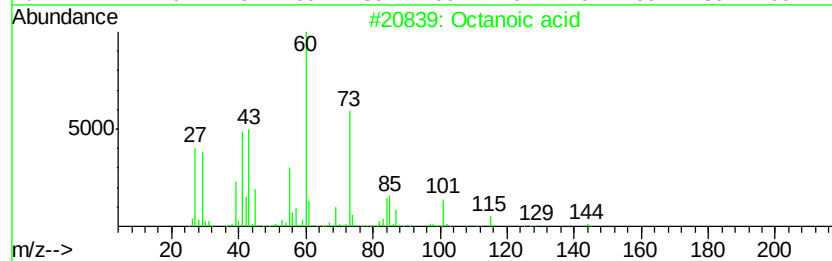
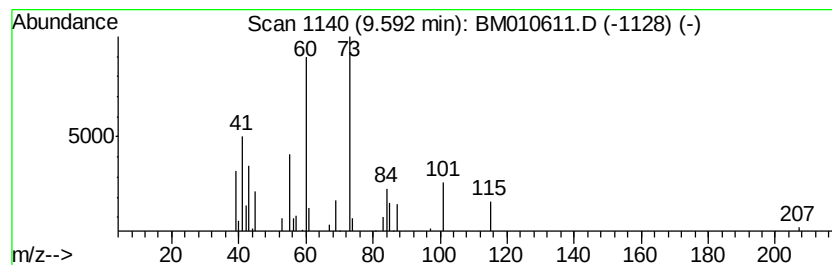
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Octanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.59	3.40 ng/ul	117473	Naphthalene-d8	10.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanoic acid	144	C8H16O2	000124-07-2	72
2		Dodecanoic acid	200	C12H24O2	000143-07-7	59
3		Undecanoic acid	186	C11H22O2	000112-37-8	59
4		Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	59
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



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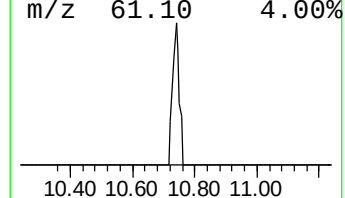
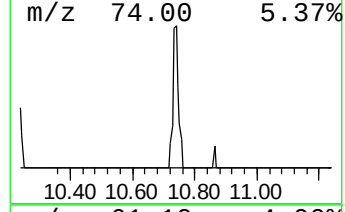
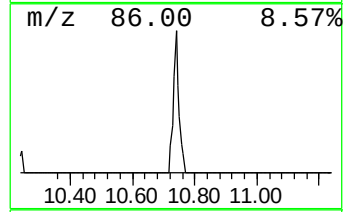
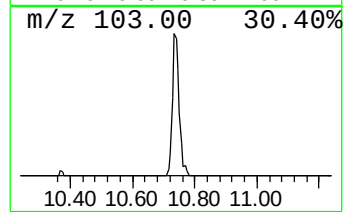
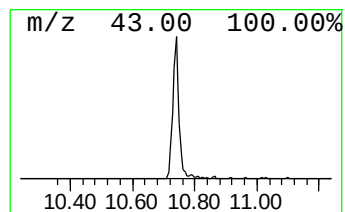
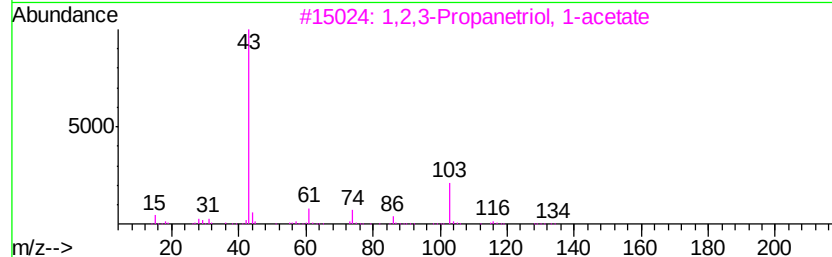
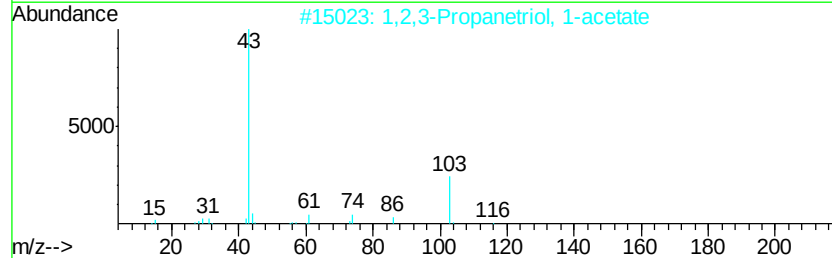
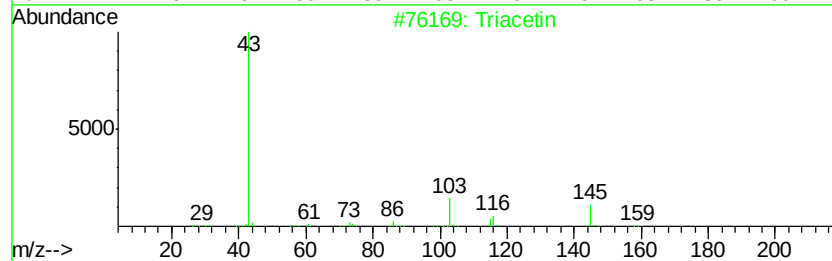
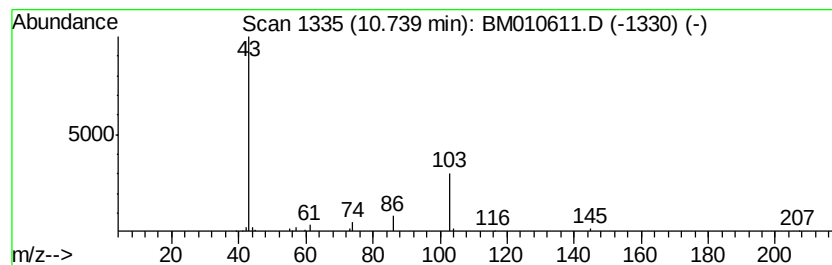
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Triacetin Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.56 ng/ul	88306	Napthalene-d8	10.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Triacetin	218 C9H14O6	000102-76-1 56
2		1,2,3-Propanetriol, 1-acetate	134 C5H10O4	000106-61-6 45
3		1,2,3-Propanetriol, 1-acetate	134 C5H10O4	000106-61-6 45
4		Triacetin	218 C9H14O6	000102-76-1 9
5		Glycerol 1,2-diacetate	176 C7H12O5	000102-62-5 9



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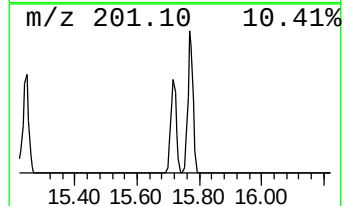
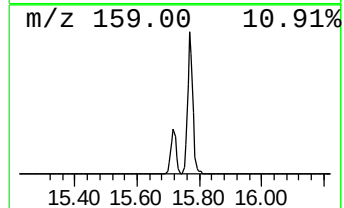
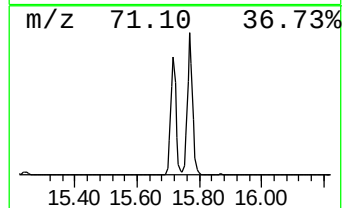
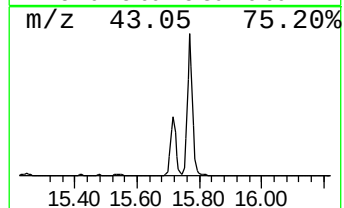
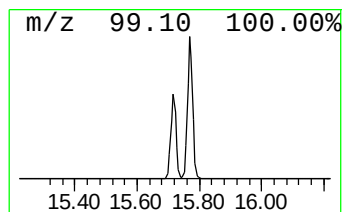
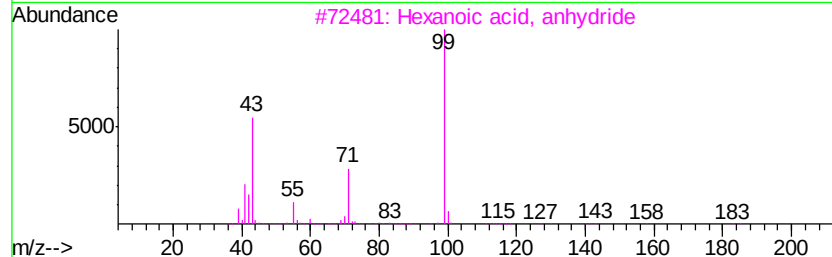
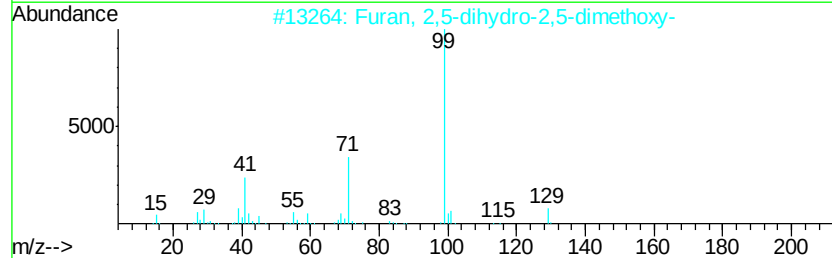
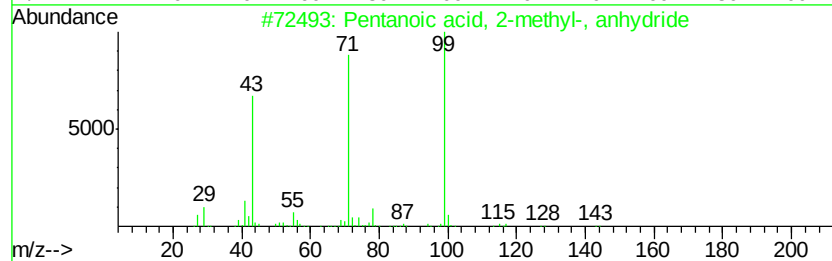
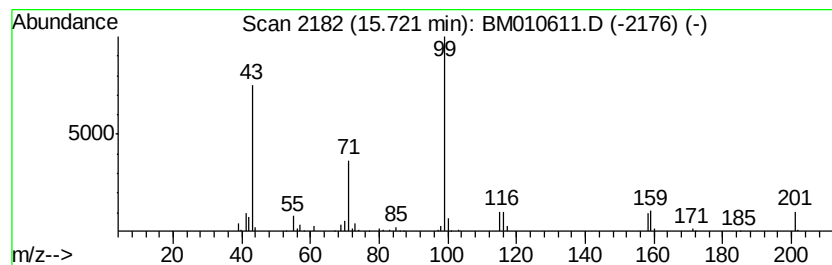
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Pentanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.72	4.67 ng/ul	324920	Phenanthrene-d10	16.87		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentanoic acid, 2-methyl-, anhyd...	214	C12H22O3	063169-61-9	53
2		Furan, 2,5-dihydro-2,5-dimethoxy-	130	C6H10O3	000332-77-4	50
3		Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	50
4		4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	50
5		Ethyl 4-(ethyloxy)-2-oxobut-3-en...	172	C8H12O4	1000305-38-2	50



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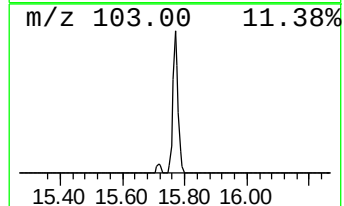
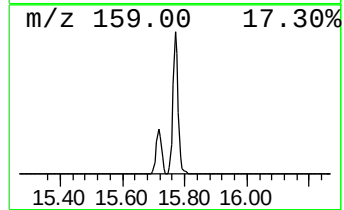
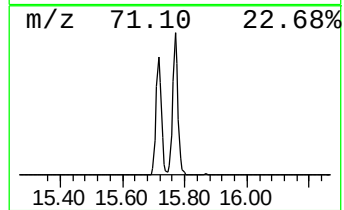
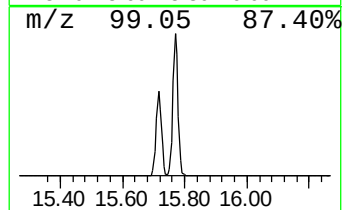
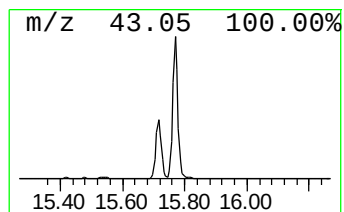
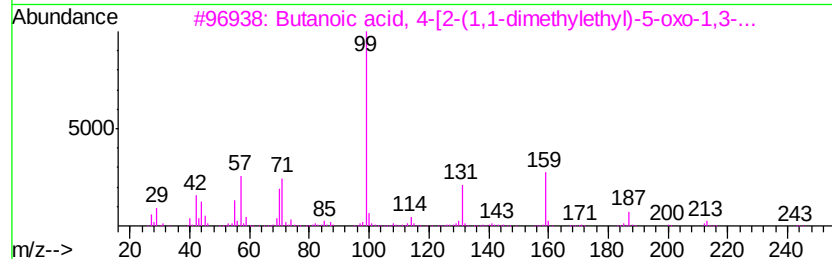
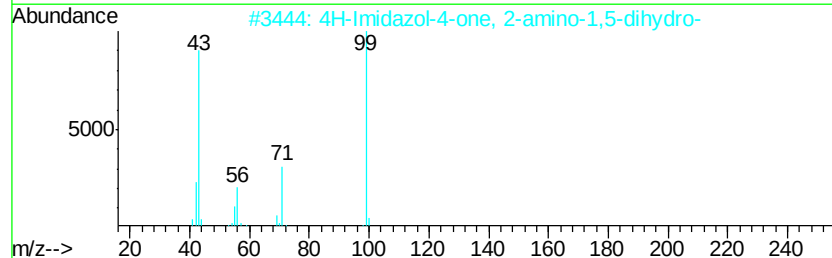
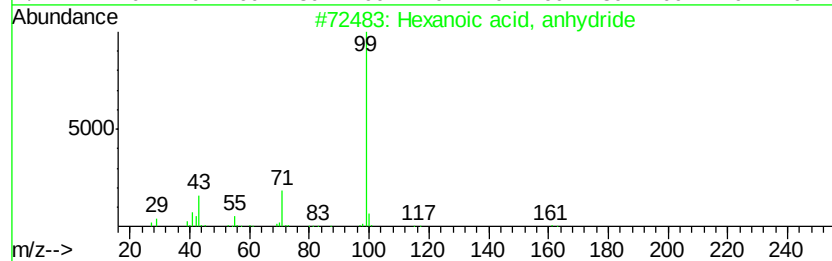
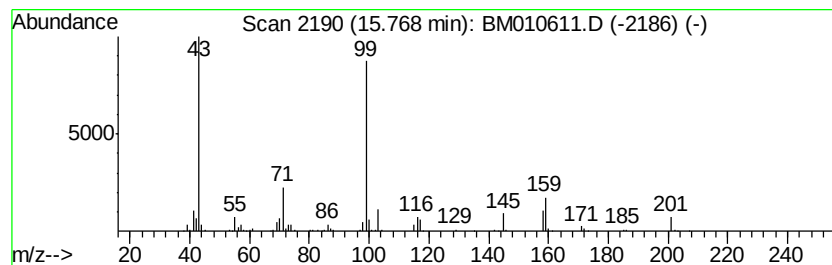
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Peak Number 4 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	9.41 ng/ul	654433	Phenanthrene-d10	16.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	47
2		4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	46
3		Butanoic acid, 4-[2-(1,1-dimethy...	244	C12H20O5	1000196-81-8	42
4		Hexanoic acid, 4-tridecyl ester	298	C19H38O2	1000279-29-3	42
5		Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	42



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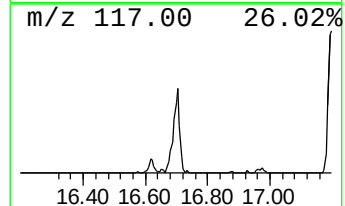
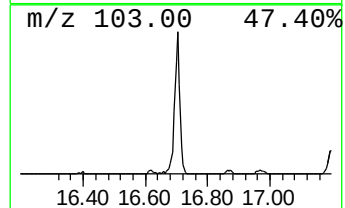
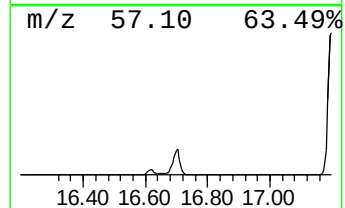
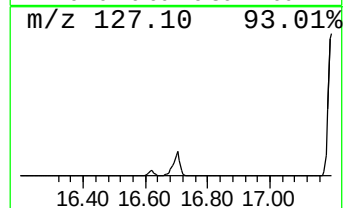
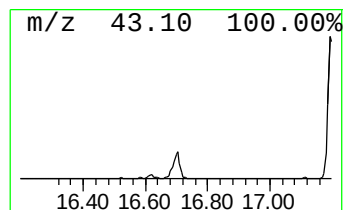
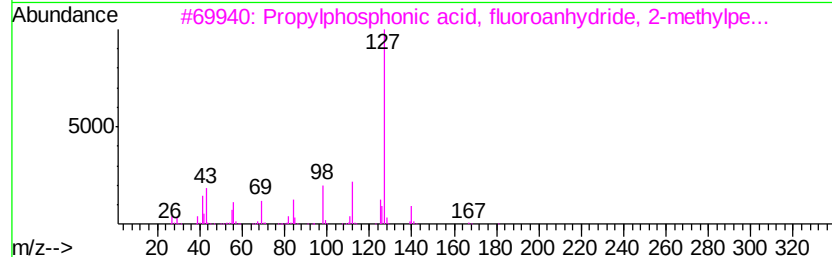
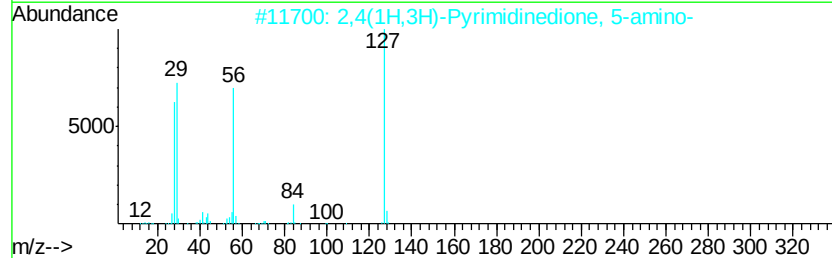
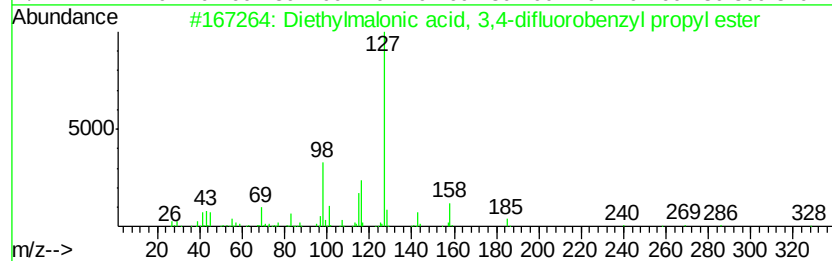
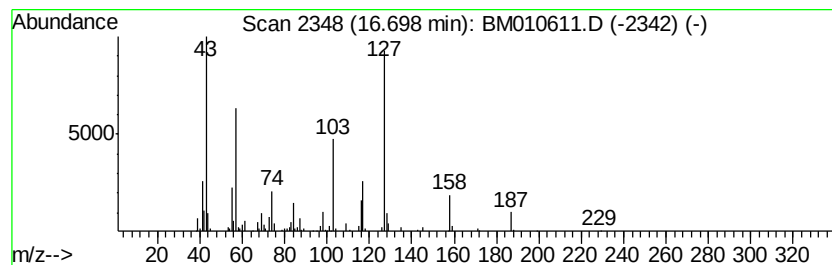
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.70	8.74 ng/ul	607516	Phenanthrene-d10	16.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylmalonic acid, 3,4-difluor...	328	C17H22F2O4	1000369-32-3	37
2	2,4(1H,3H)-Pyrimidinedione, 5-am...	127	C4H5N3O2	000932-52-5	35
3	Propylphosphonic acid, fluoroanh...	210	C9H20F02P	333416-27-6	35
4	Caprylic anhydride	270	C16H30O3	000623-66-5	32
5	Octanoic acid, 2-octyl ester	256	C16H32O2	055193-33-4	25



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010611.D
Acq On : 21 Jun 2017 03:54
Operator : SJ/MA
Sample : I3790-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

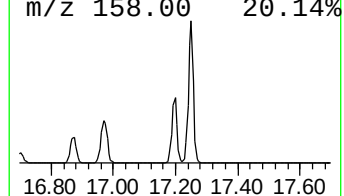
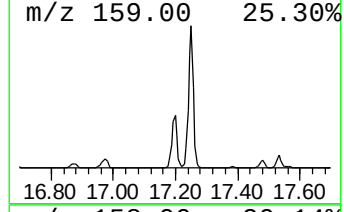
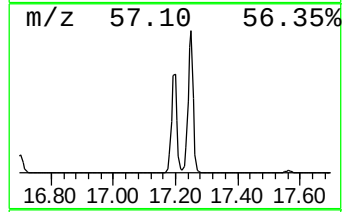
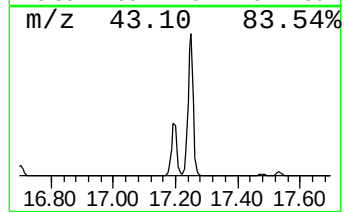
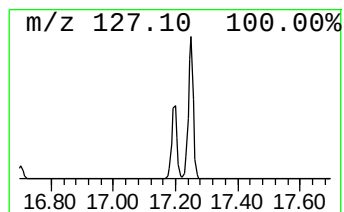
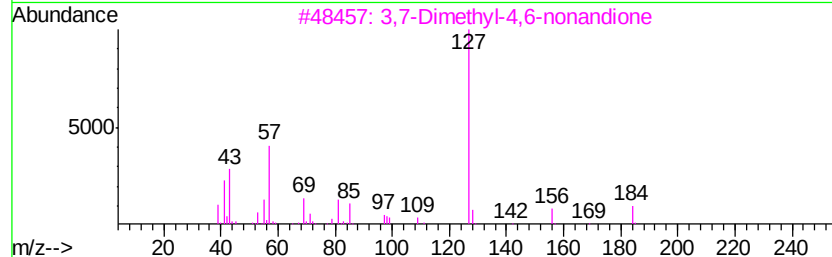
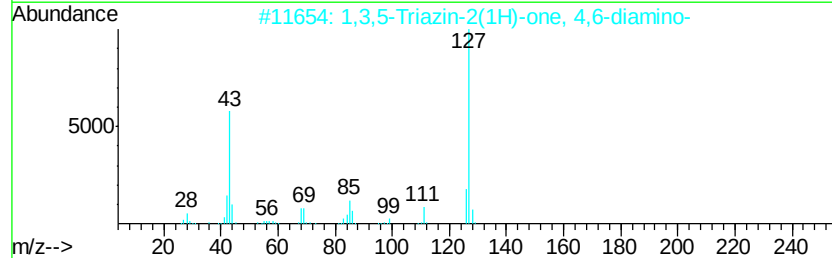
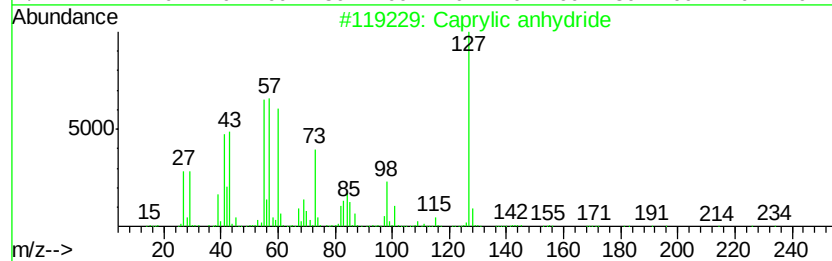
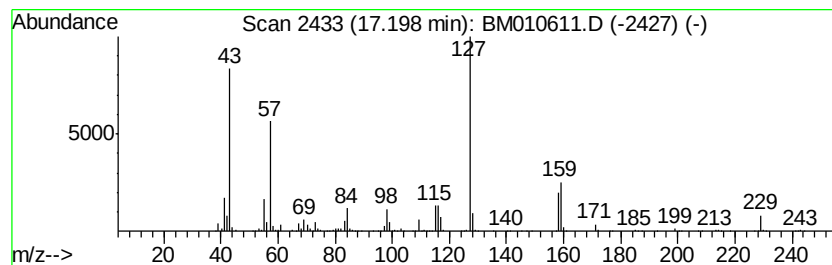
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.20	33.23 ng/ul	2310130	Phenanthrene-d10	16.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Caprylic anhydride	270 C16H30O3	000623-66-5 47
2		1,3,5-Triazin-2(1H)-one, 4,6-dia...	127 C3H5N5O	000645-92-1 43
3		3,7-Dimethyl-4,6-nonandione	184 C11H20O2	1000374-12-6 43
4		1,3-Benzenediol, 0-dichloroacety...	346 C16H20Cl2O4	1000345-48-0 43
5		Octanoic acid, 3-fluorophenyl ester	238 C14H19FO2	1000330-94-7 43



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
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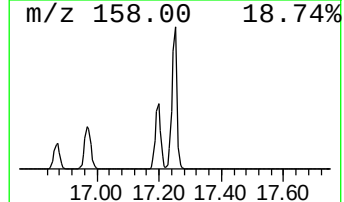
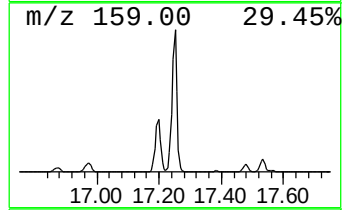
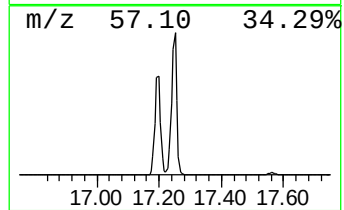
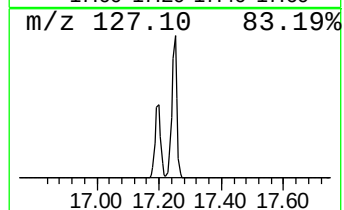
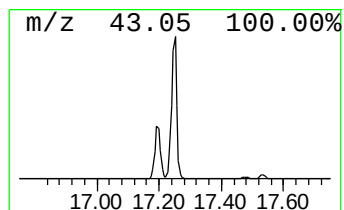
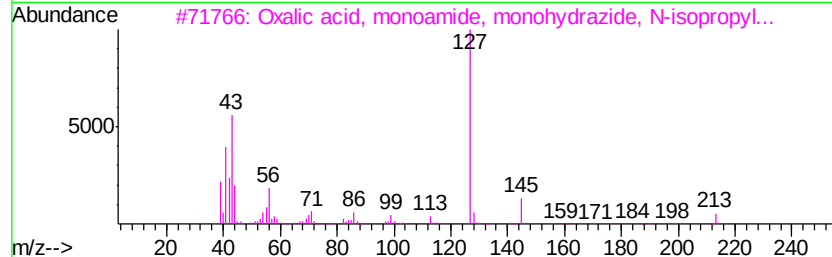
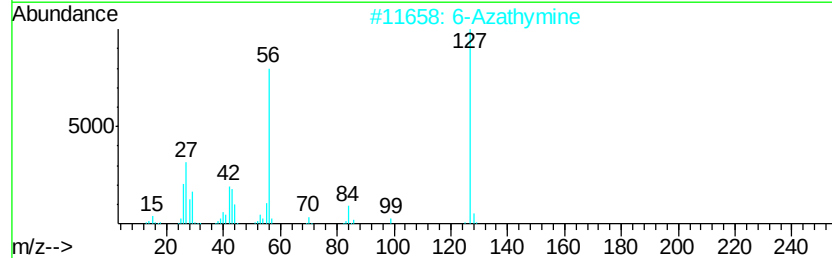
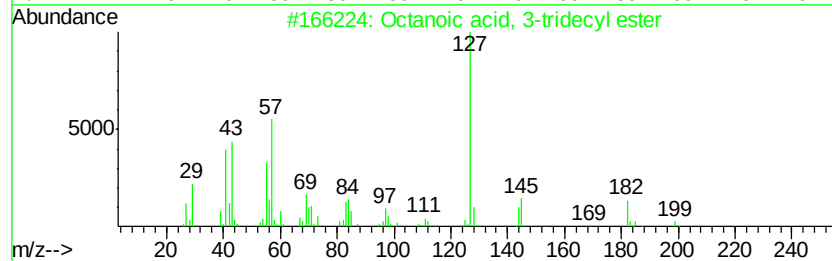
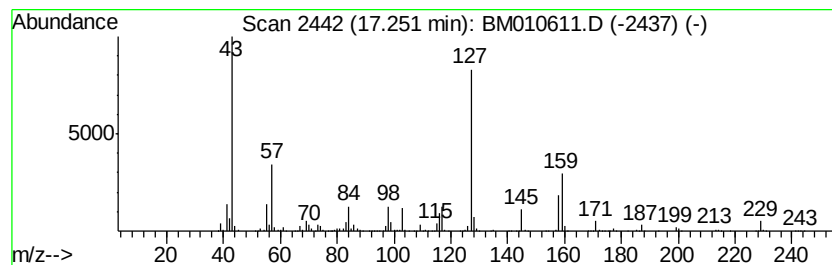
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.25	71.90 ng/ul	4998850	Phenanthrene-d10	16.87		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octanoic acid, 3-tridecyl ester	326	C21H42O2	1000280-62-5	38
2		6-Azathymine	127	C4H5N3O2	000932-53-6	32
3		Oxalic acid, monoamide, monohydr...	213	C10H19N3O2	1000265-20-0	32
4		Caprylic anhydride	270	C16H30O3	000623-66-5	32
5		Phosphonofluoridic acid, propyl-...	252	C12H26F02P	333416-21-0	32



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010611.D
Acq On : 21 Jun 2017 03:54
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Sample : I3790-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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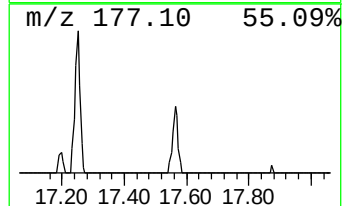
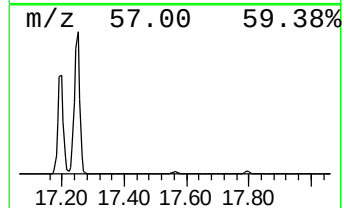
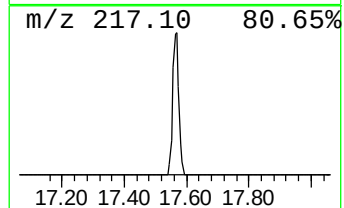
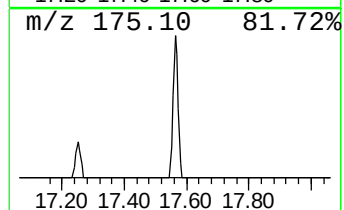
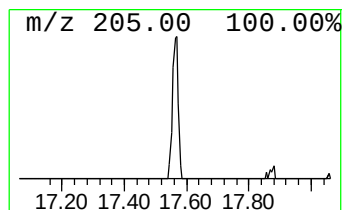
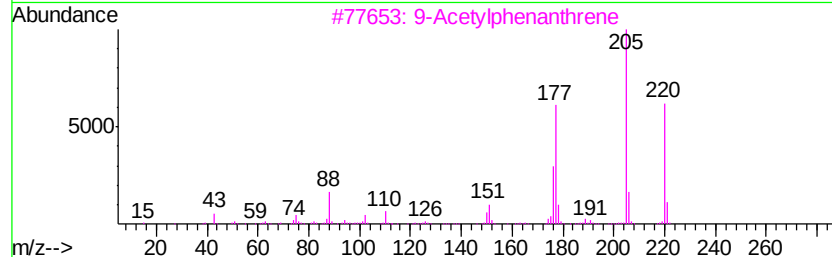
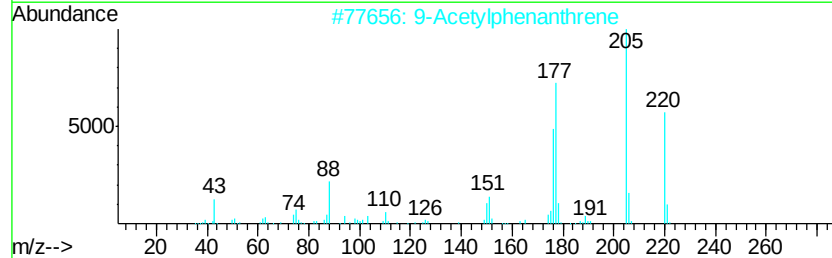
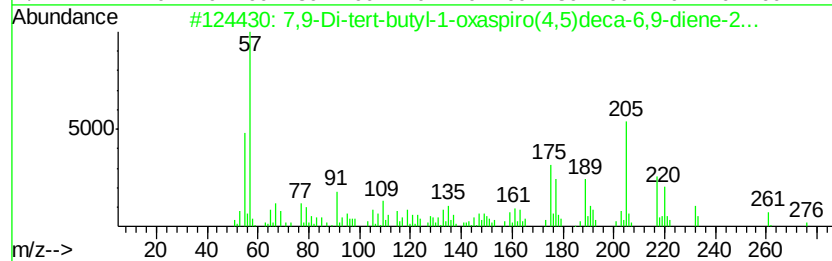
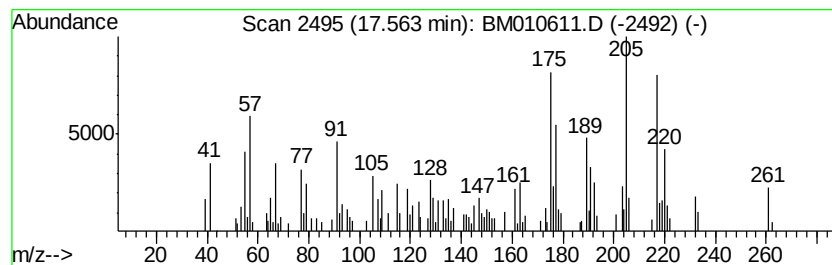
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.56	2.14 ng/ul	148608	Phenanthrene-d10	16.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	68
2			9-Acetylphenanthrene	220	C16H12O	002039-77-2	42
3			9-Acetylphenanthrene	220	C16H12O	002039-77-2	38
4			1-Ethyl-2-methylphenanthrene	220	C17H16	061983-53-7	35
5			3-Acetylphenanthrene	220	C16H12O	002039-76-1	30



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
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Misc :
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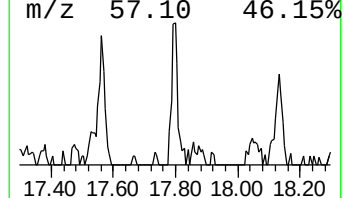
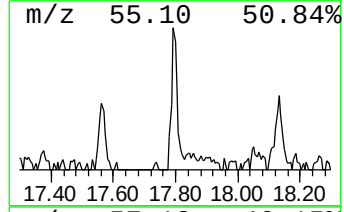
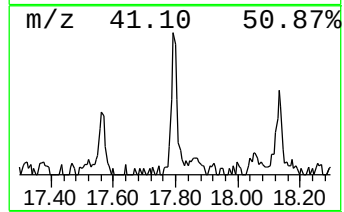
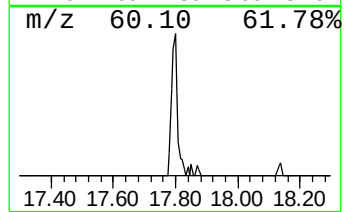
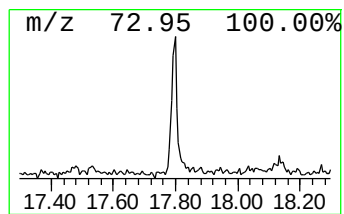
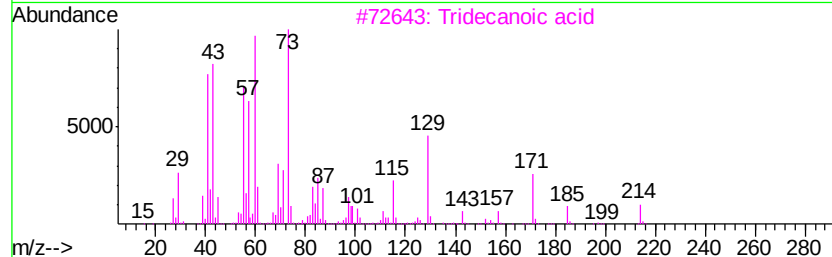
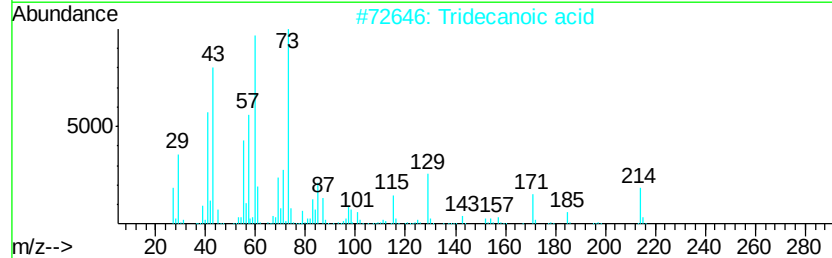
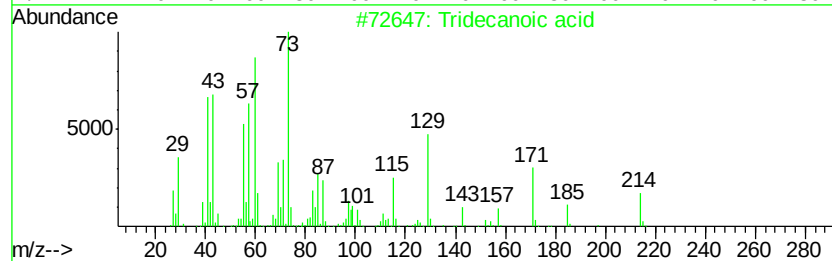
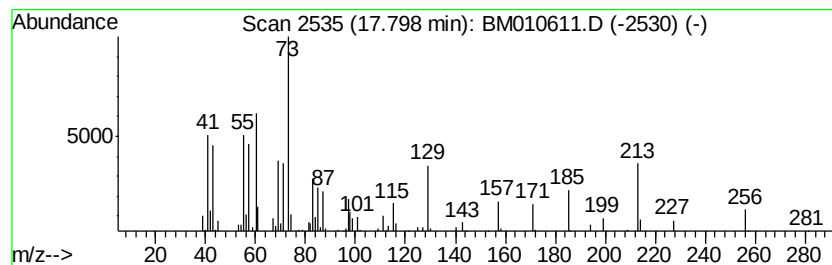
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 Tridecanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.80	2.34 ng/ul	162946	Phenanthrene-d10	16.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Tridecanoic acid	214 C13H26O2	000638-53-9	93
2	Tridecanoic acid	214 C13H26O2	000638-53-9	92
3	Tridecanoic acid	214 C13H26O2	000638-53-9	90
4	n-Hexadecanoic acid	256 C16H32O2	000057-10-3	64
5	Tridecanoic acid	214 C13H26O2	000638-53-9	60



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010611.D
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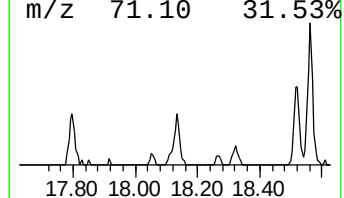
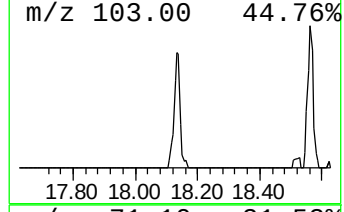
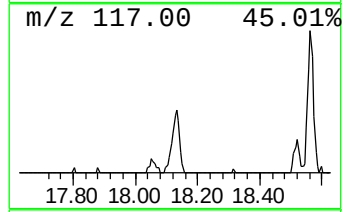
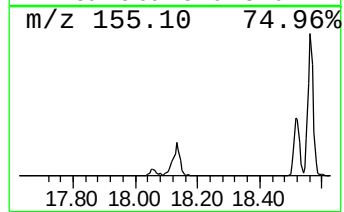
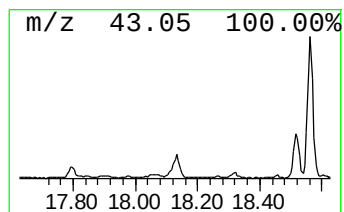
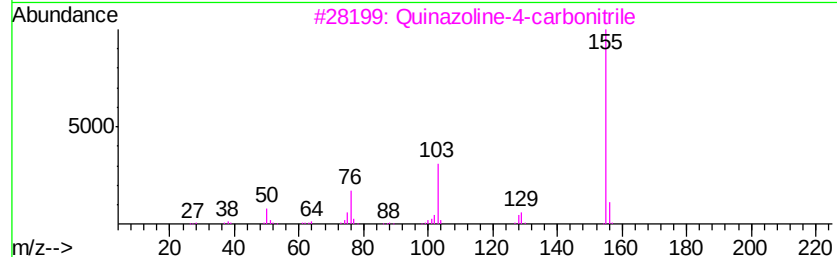
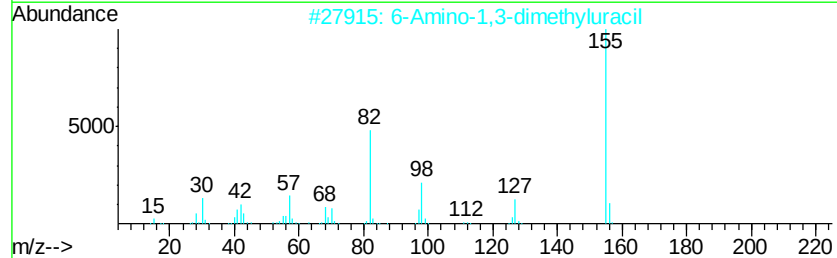
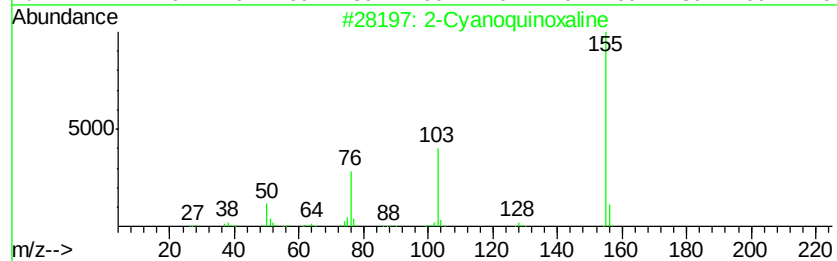
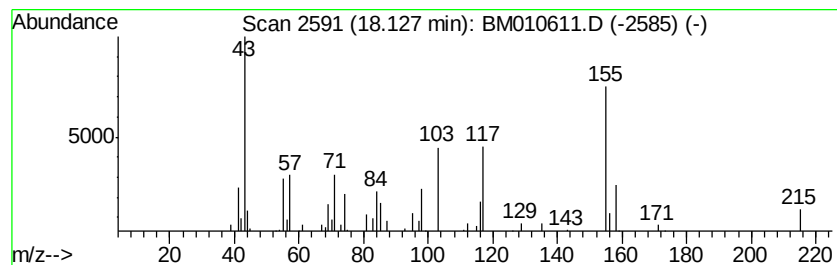
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 unknown-05 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.13	2.06 ng/ul	143197	Phenanthrene-d10	16.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyanoquinoxaline	155	C9H5N3	007483-33-2	38
2			6-Amino-1,3-dimethyluracil	155	C6H9N3O2	006642-31-5	35
3			Quinazoline-4-carbonitrile	155	C9H5N3	036082-71-0	27
4			1,3,5-Triazin-2(1H)-one, 4,6-bis...	155	C5H9N5O	055702-52-8	25
5			Fumaric acid, butyl isobutyl ester	228	C12H20O4	1000330-37-3	25



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
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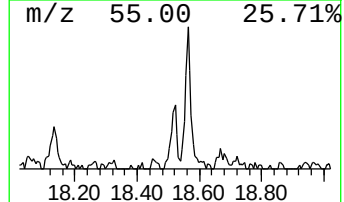
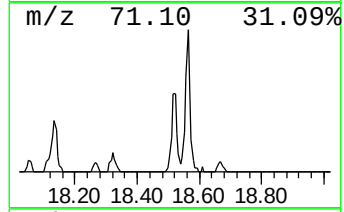
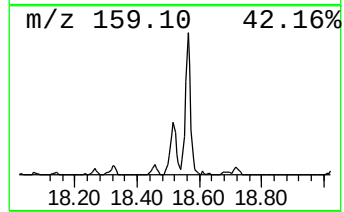
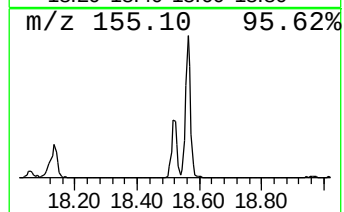
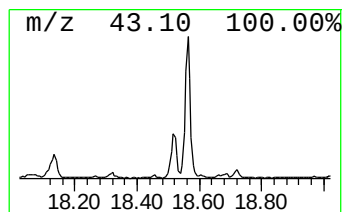
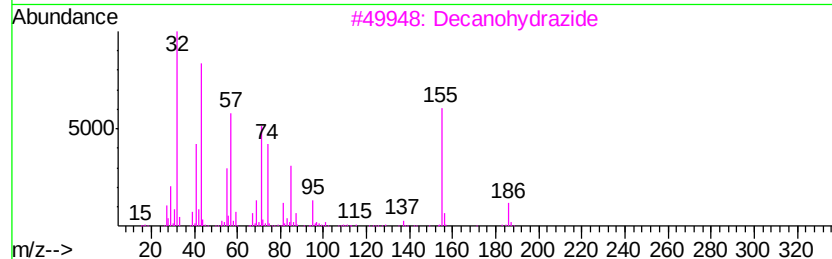
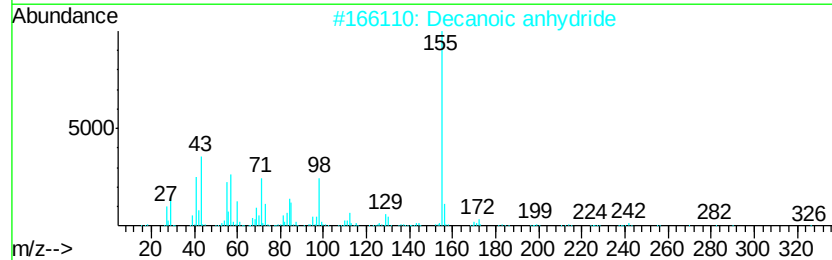
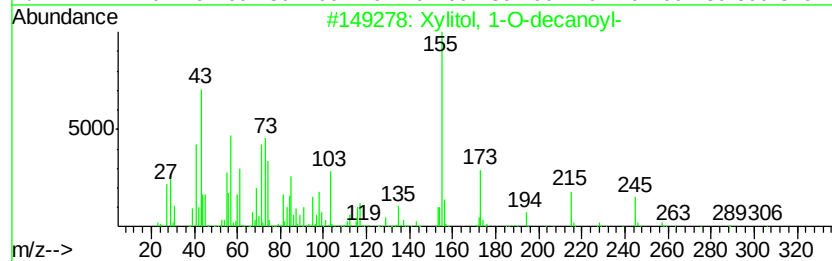
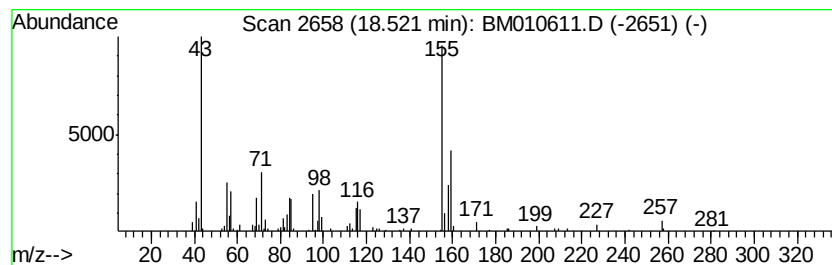
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 unknown-06 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.52	2.84 ng/ul	197223	Phenanthrene-d10		16.87
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Xylitol, 1-O-decanoyl-	306	C15H30O6	1000155-78-0	42
2	Decanoic anhydride	326	C20H38O3	002082-76-0	40
3	Decanohydrazide	186	C10H22N2O	020478-70-0	37
4	Vinyl decanoate	198	C12H22O2	004704-31-8	37
5	[1,1'-Bicyclohexyl]-1,1'-diol, 3...	310	C20H38O2	068525-22-4	27



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
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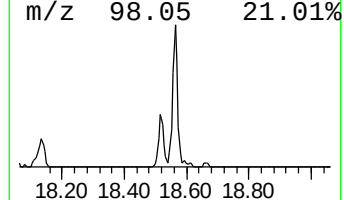
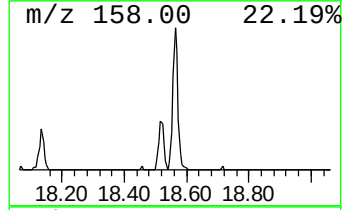
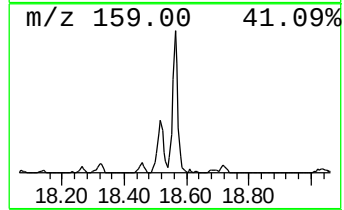
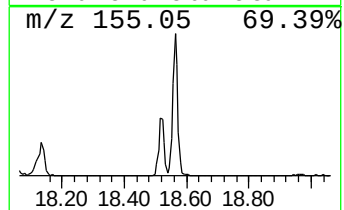
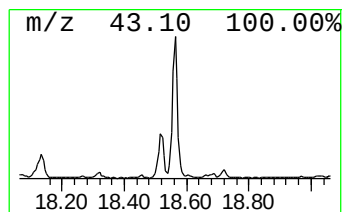
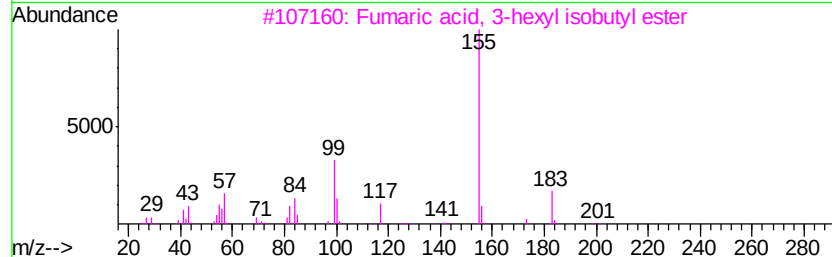
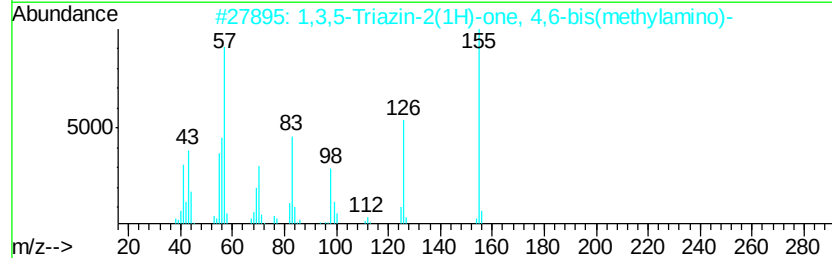
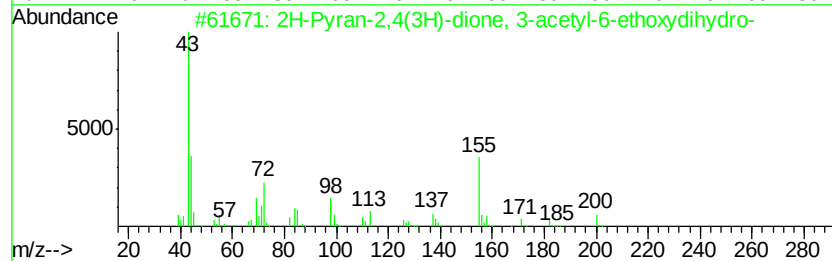
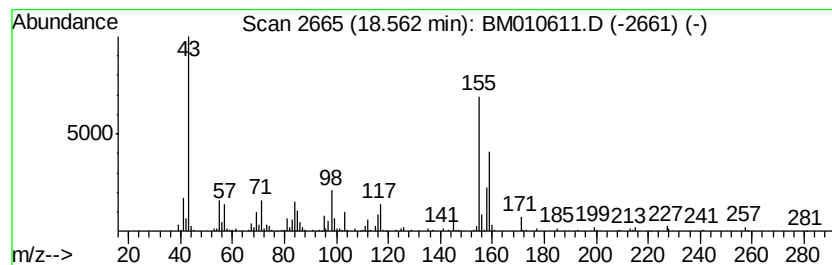
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Quant Title : SVOA CALIBRATION

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

Peak Number 12 unknown-07 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.56	6.71 ng/ul	466512	Phenanthrene-d10	16.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Pyran-2,4(3H)-dione, 3-acetyl...	200	C9H12O5	1000318-74-8	37
2			1,3,5-Triazin-2(1H)-one, 4,6-bis...	155	C5H9N5O	055702-52-8	27
3			Fumaric acid, 3-hexyl isobutyl e...	256	C14H24O4	1000348-60-3	27
4			6-Amino-1,3-dimethyluracil	155	C6H9N3O2	006642-31-5	22
5			Fumaric acid, butyl 3-heptyl ester	270	C15H26O4	1000348-68-0	22



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010611.D
Acq On : 21 Jun 2017 03:54
Operator : SJ/MA
Sample : I3790-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0B84

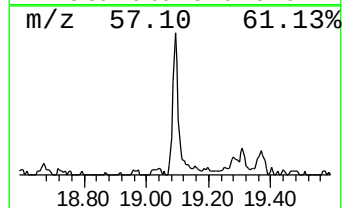
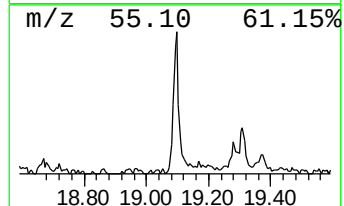
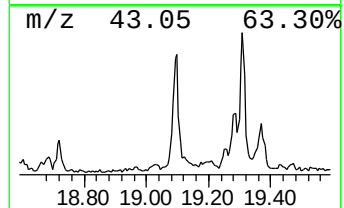
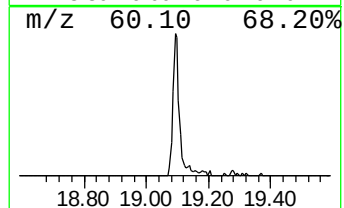
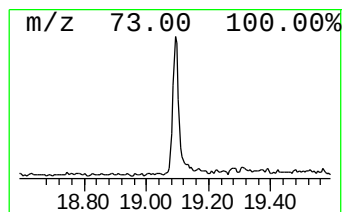
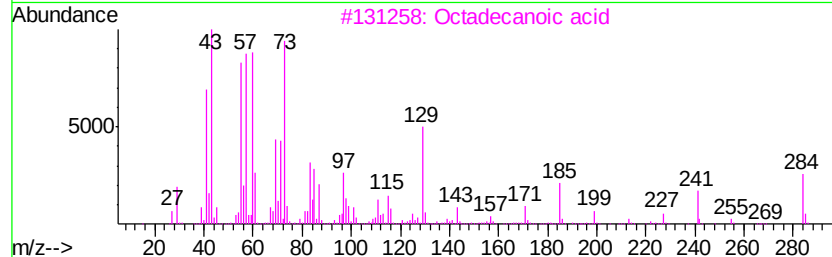
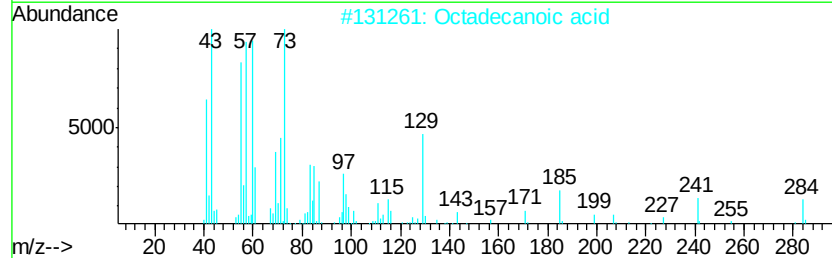
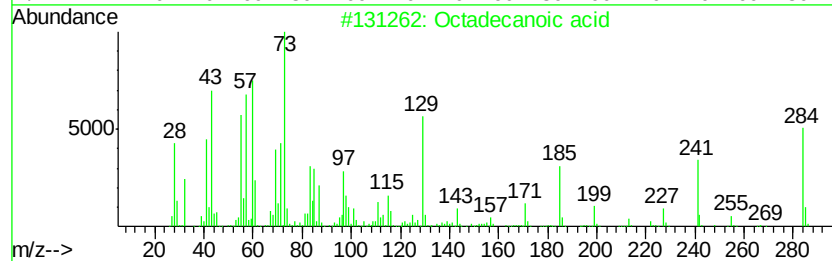
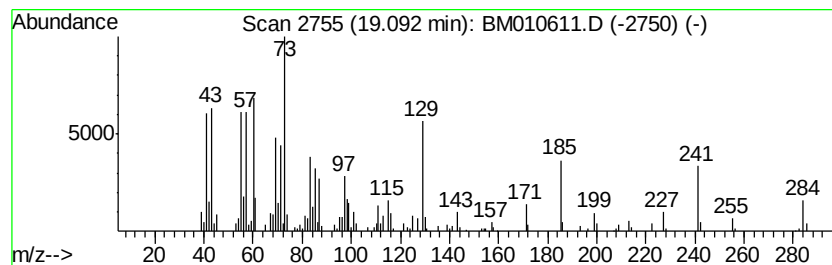
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Quant Title : SVOA CALIBRATION

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

Peak Number 13 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.09	4.33 ng/ul	406505	Chrysene-d12	21.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid	284	C18H36O2	000057-11-4	96
3		Octadecanoic acid	284	C18H36O2	000057-11-4	96
4		Octadecanoic acid	284	C18H36O2	000057-11-4	96
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	78



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010611.D
Acq On : 21 Jun 2017 03:54
Operator : SJ/MA
Sample : I3790-12
Misc :
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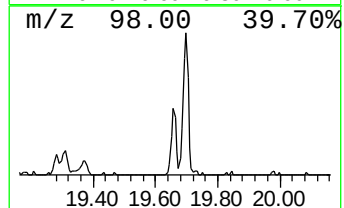
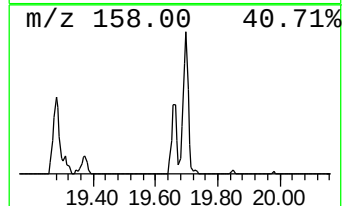
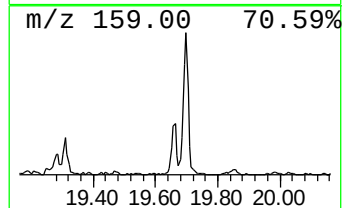
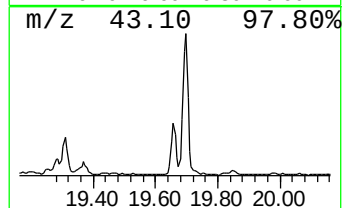
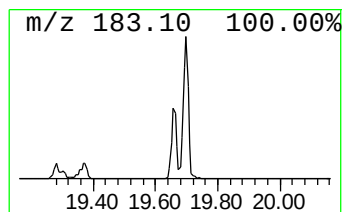
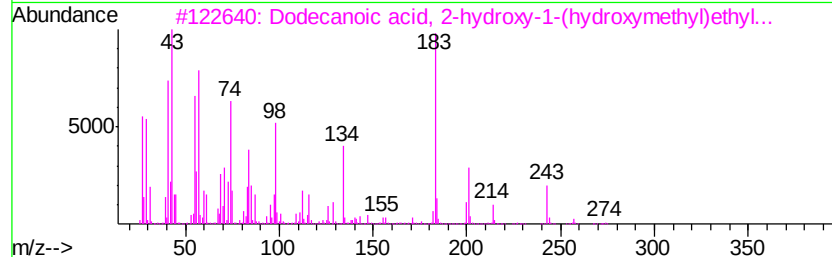
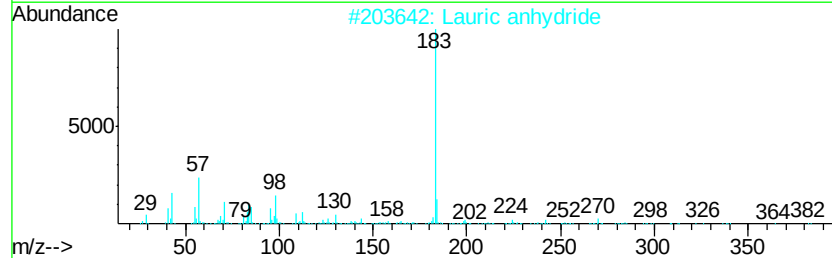
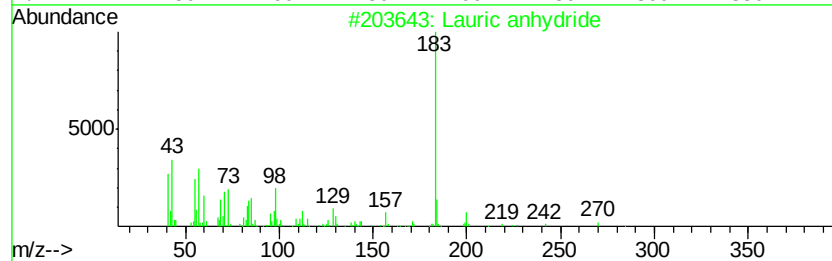
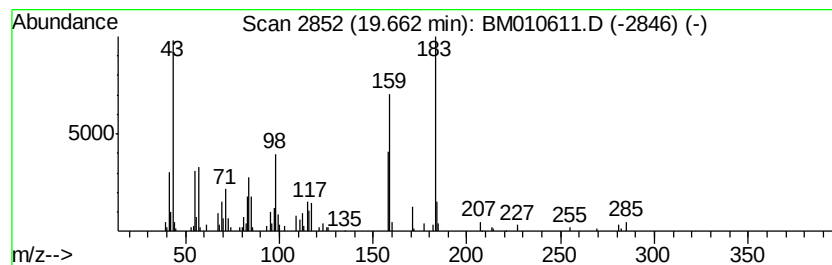
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Quant Title : SVOA CALIBRATION

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

Peak Number 14 unknown-08 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.66	2.30 ng/ul	215880	Chrysene-d12	21.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Lauric anhydride	382 C24H46O3	000645-66-9	43
2	Lauric anhydride	382 C24H46O3	000645-66-9	43
3	Dodecanoic acid, 2-hydroxy-1-(hy...	274 C15H30O4	001678-45-1	40
4	Hexadecanoic acid, 2,3-bis(acety...	414 C23H42O6	055268-70-7	38
5	Fumaric acid, cyclobutyl isohexy...	254 C14H22O4	1000345-03-5	35



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010611.D
Acq On : 21 Jun 2017 03:54
Operator : SJ/MA
Sample : I3790-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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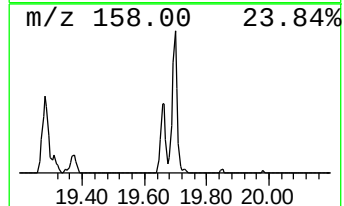
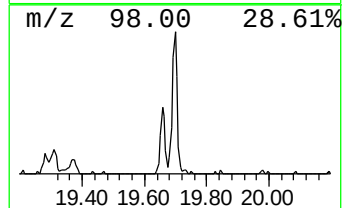
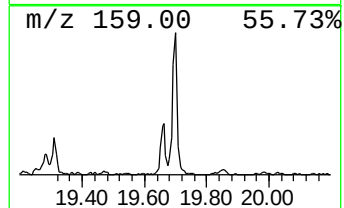
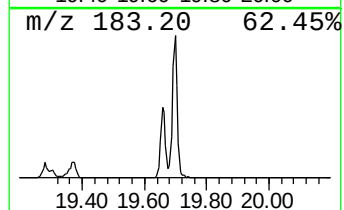
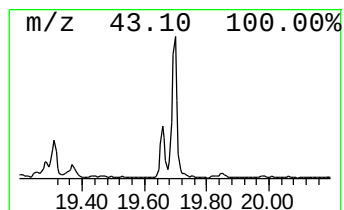
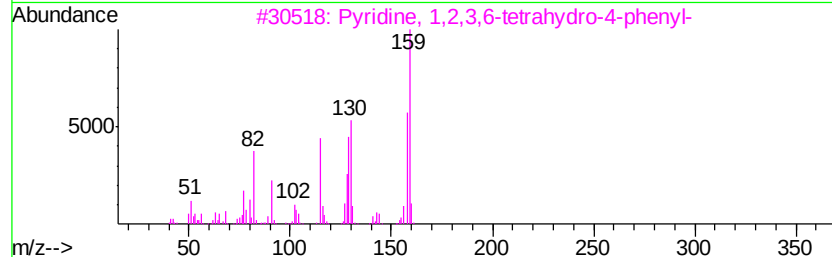
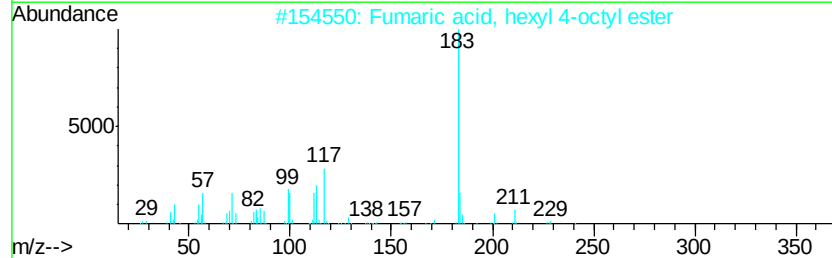
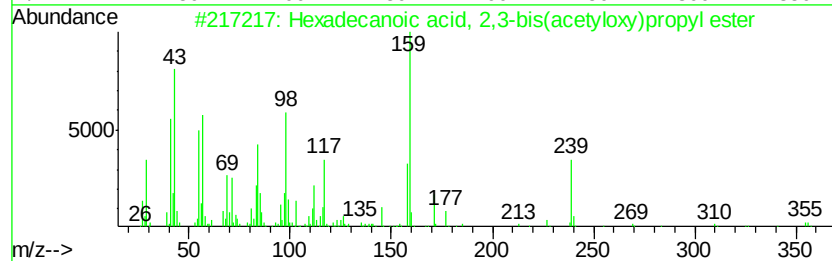
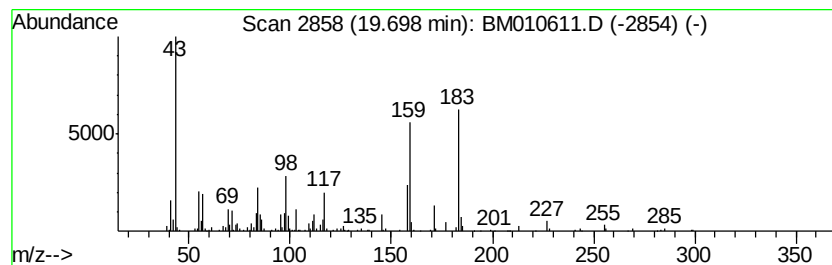
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Quant Title : SVOA CALIBRATION

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

Peak Number 15 Hexadecanoic acid, 2,3-bis(...) Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.70	5.31 ng/ul	499005	Chrysene-d12	21.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	62
2		Fumaric acid, hexyl 4-octyl ester	312	C18H32O4	1000339-21-7	14
3		Pyridine, 1,2,3,6-tetrahydro-4-p...	159	C11H13N	010338-69-9	14
4		Lauric anhydride	382	C24H46O3	000645-66-9	12
5		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	12



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
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Acq On : 21 Jun 2017 03:54
Operator : SJ/MA
Sample : I3790-12
Misc :
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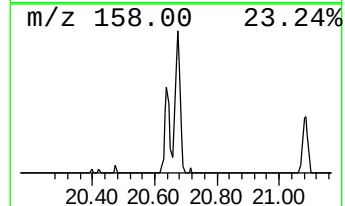
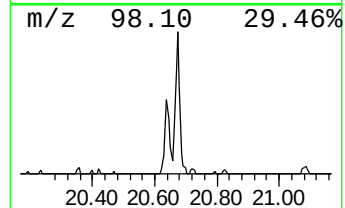
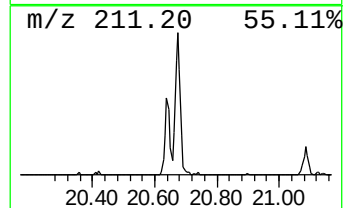
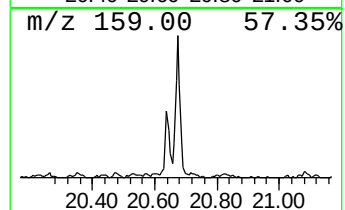
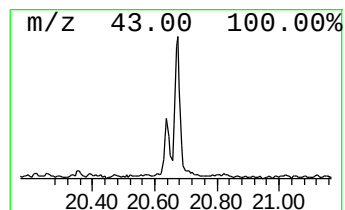
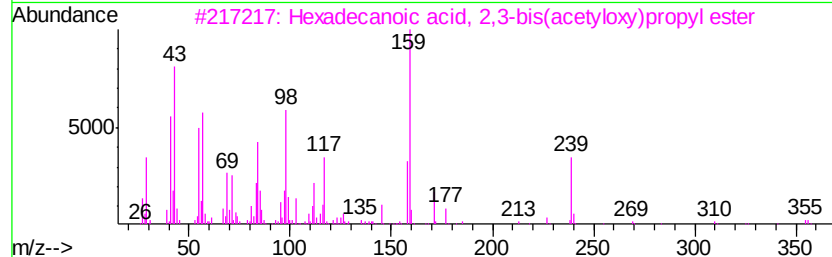
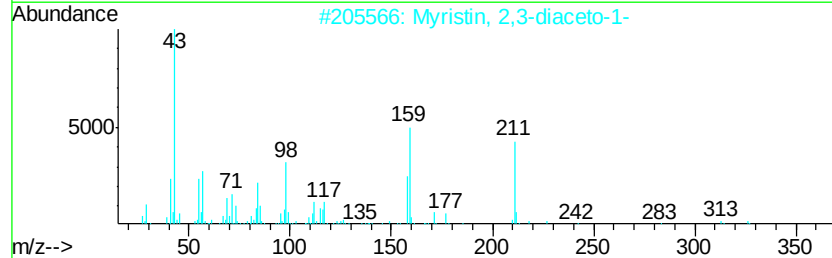
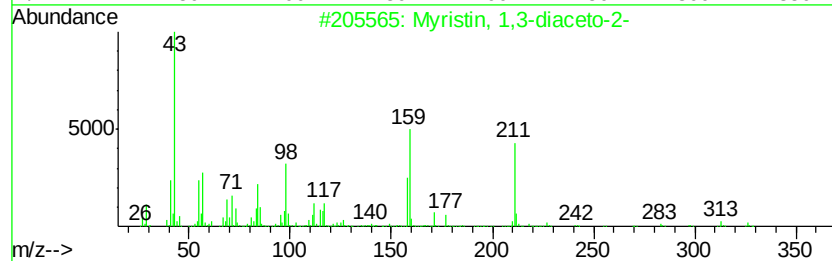
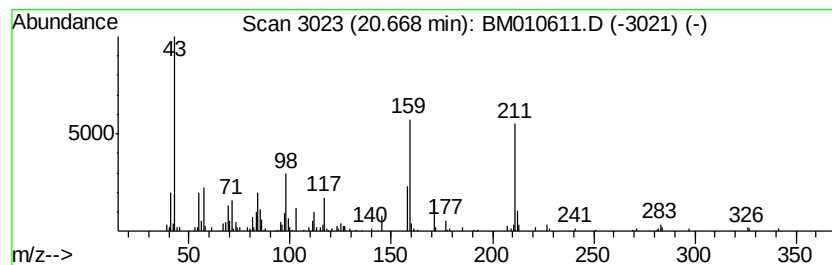
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 16 Myristin, 1,3-diaceto-2- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.		
20.67	3.39 ng/ul	318109	Chrysene-d12	21.09		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	53	
2	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	53	
3	Hexadecanoic acid, 2,3-bis(acetyloxy)propyl ester	414	C23H42O6	055268-70-7	49	
4	Eicosanoic acid, 2,3-bis(acetyloxy)propyl ester	470	C27H50O6	055429-67-9	27	
5	2,3,4-Trifluorobenzoic acid, 4-methyl-1,3-dioxane-5-carboxylate	260	C13H15F3O2	1000282-29-8	27	



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010611.D
Acq On : 21 Jun 2017 03:54
Operator : SJ/MA
Sample : I3790-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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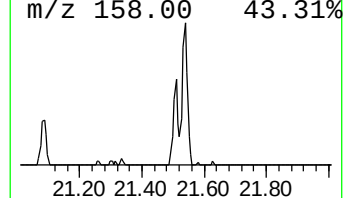
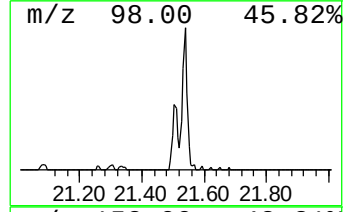
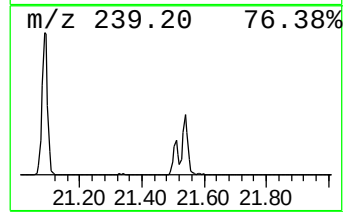
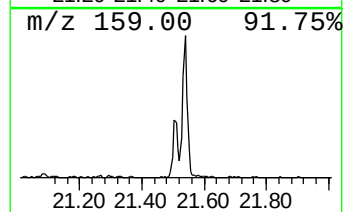
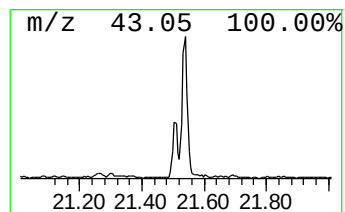
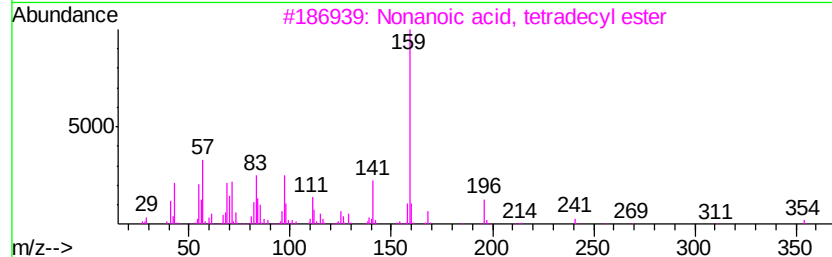
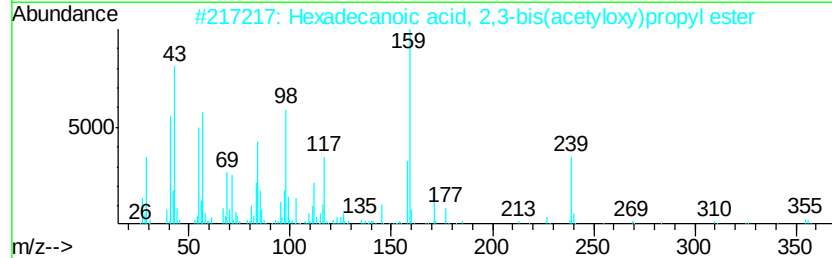
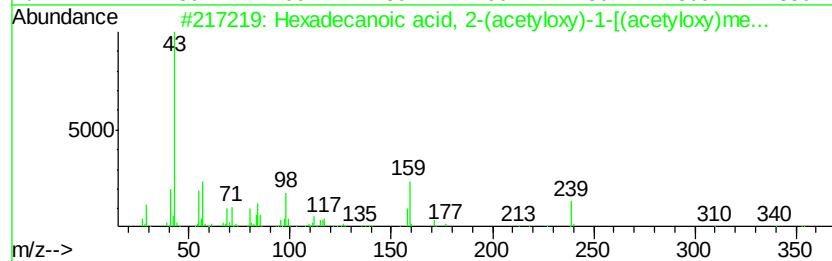
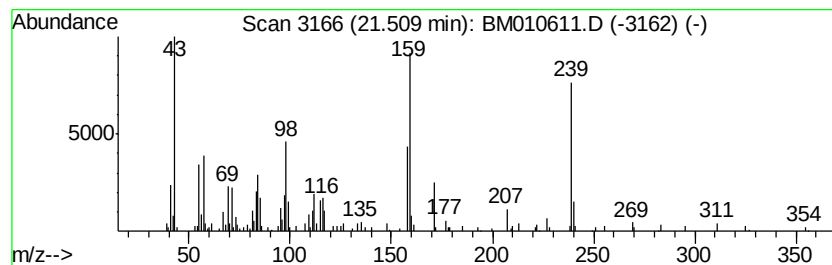
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Quant Title : SVOA CALIBRATION

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

Peak Number 17 Hexadecanoic acid, 2-(acety... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.51	2.19 ng/ul	205283	Chrysene-d12	21.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	86
2		Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	83
3		Nonanoic acid, tetradecyl ester	354	C23H46O2	1000340-28-1	47
4		4,6-Difluoro-2-dimethylaminopyri...	159	C6H7F2N3	165258-63-9	25
5		1-Methyl-2-formylindole	159	C10H9NO	027421-51-8	22



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
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Sample : I3790-12
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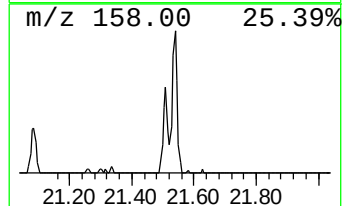
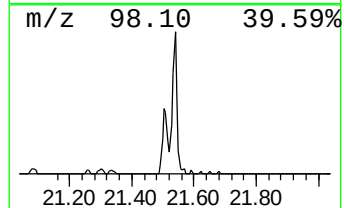
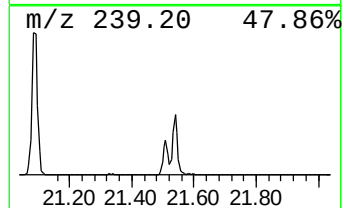
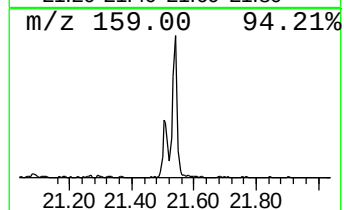
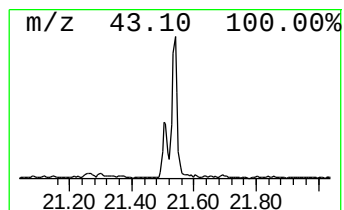
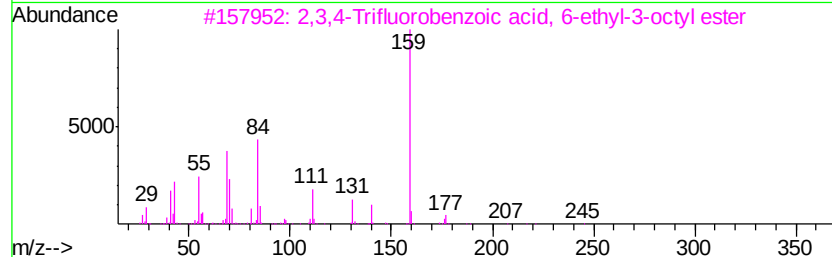
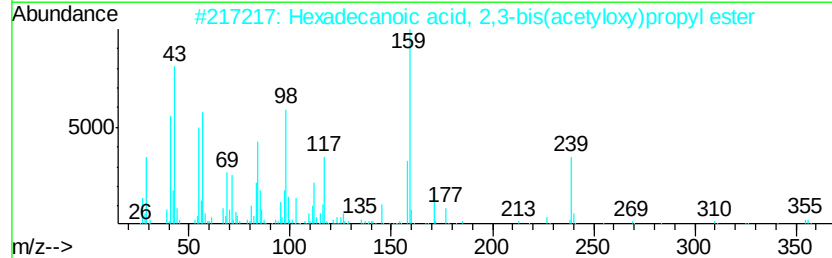
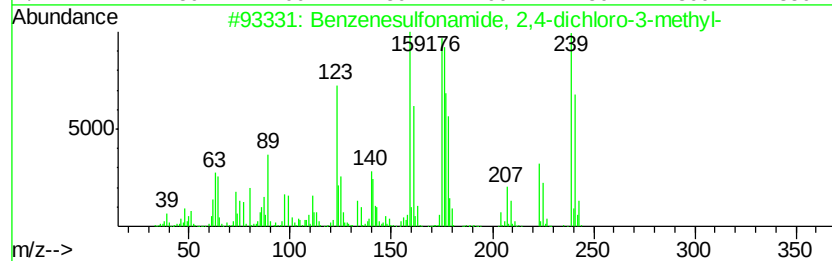
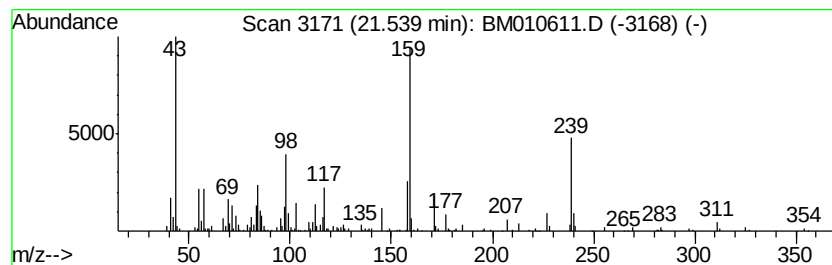
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Quant Title : SVOA CALIBRATION

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

Peak Number 18 unknown-09 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.54	4.37 ng/ul	410300	Chrysene-d12	21.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzenesulfonamide, 2,4-dichloro...	239 C7H7Cl2N02S	1000277-29-3 43
2		Hexadecanoic acid, 2,3-bis(acety...	414 C23H42O6	055268-70-7 38
3		2,3,4-Trifluorobenzoic acid, 6-e...	316 C17H23F3O2	1000282-58-3 27
4		Diethylmalonic acid, hexyl 4-tri...	402 C21H29F3O4	1000368-40-4 25
5		2,6-Difluorobenzoic acid, octade...	410 C25H40F2O2	1000292-39-7 22



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
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Acq On : 21 Jun 2017 03:54
Operator : SJ/MA
Sample : I3790-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0B84

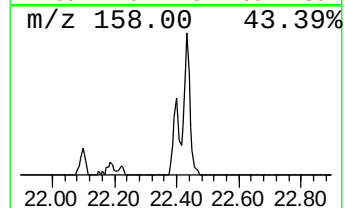
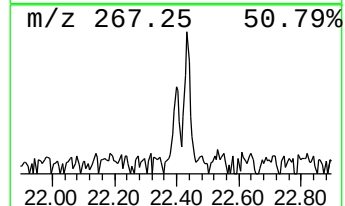
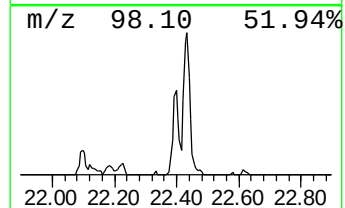
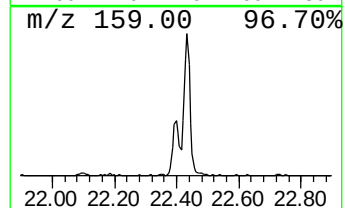
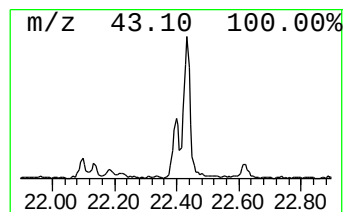
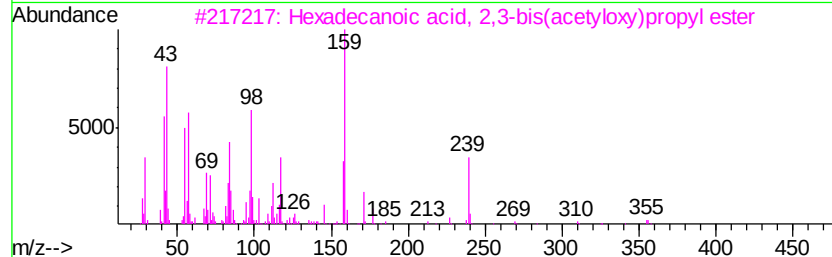
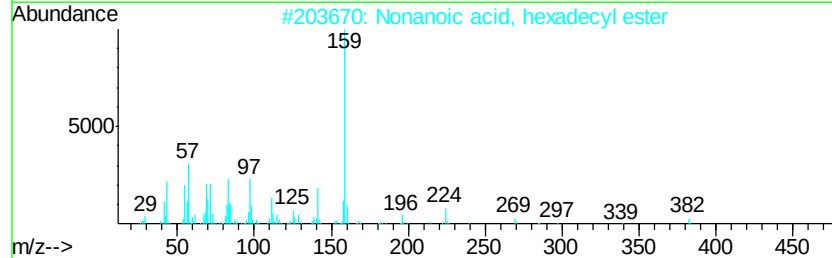
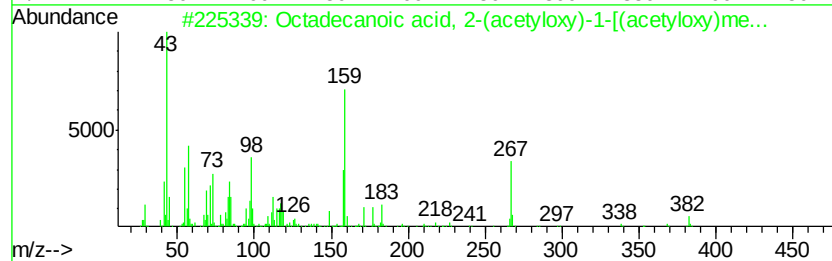
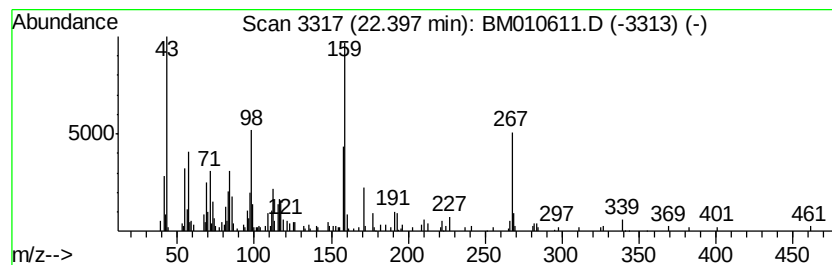
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Quant Title : SVOA CALIBRATION

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

Peak Number 19 Octadecanoic acid, 2-(acety... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.40	3.19 ng/ul	255965	Perylene-d12	23.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, 2-(acetyloxy)...	442	C25H46O6	055401-62-2	91
2		Nonanoic acid, hexadecyl ester	382	C25H50O2	1000340-28-3	55
3		Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	52
4		Stearic anhydride	551	C36H70O3	000638-08-4	38
5		Octadecanoic acid, 2,3-dihydroxy...	358	C21H42O4	000123-94-4	30



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010611.D
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Sample : I3790-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0B84

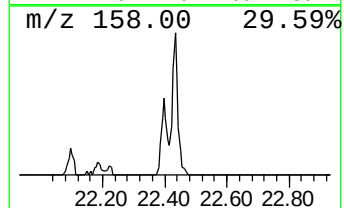
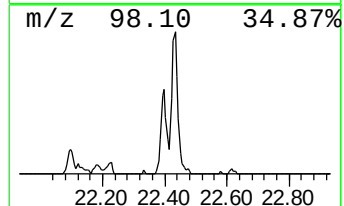
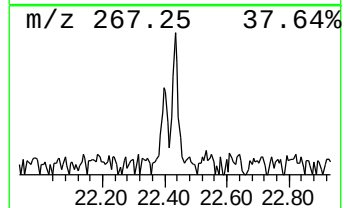
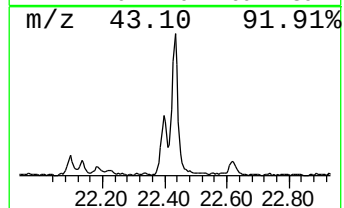
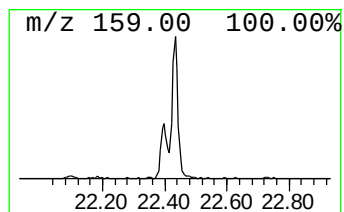
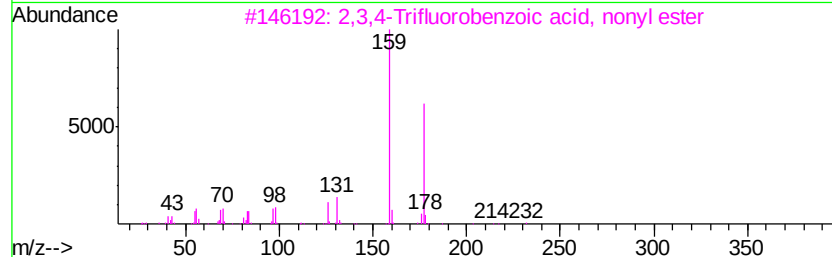
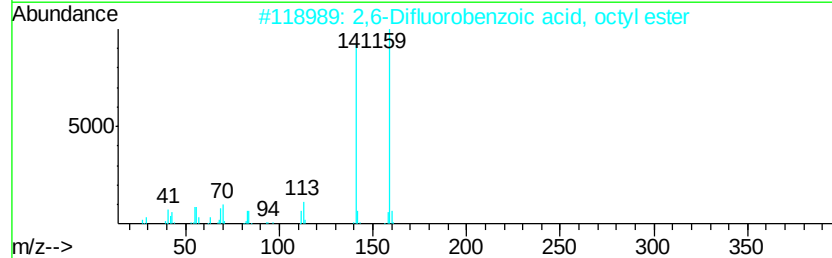
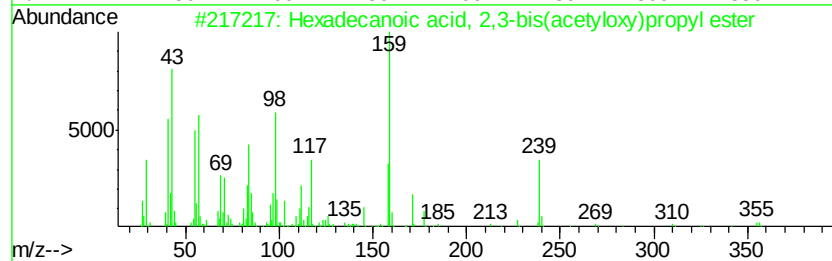
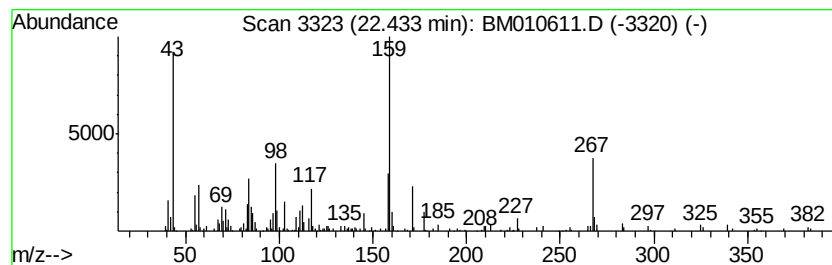
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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

Peak Number 20 unknown-10 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.43	5.74 ng/ul	461021	Perylene-d12	23.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	43
2		2,6-Difluorobenzoic acid, octyl ...	270	C15H20F2O2	1000292-39-2	35
3		2,3,4-Trifluorobenzoic acid, non...	302	C16H21F3O2	1000283-00-2	35
4		2-Naphthalenol, 1-amino-	159	C10H9NO	002834-92-6	35
5		2,3,4-Trifluorobenzoic acid, 3-t...	358	C20H29F3O2	1000280-61-8	32



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
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Instrument :
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.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
Octanoic acid	9.59	3.4	ng/ul	117473	2	10.23	690402	20.0
Triacetin	10.74	2.6	ng/ul	88306	2	10.23	690402	20.0
Pentanoic acid, 2...	15.72	4.7	ng/ul	324920	4	16.87	1390510	20.0
unknown-01	15.77	9.4	ng/ul	654433	4	16.87	1390510	20.0
unknown-02	16.70	8.7	ng/ul	607516	4	16.87	1390510	20.0
unknown-03	17.20	33.2	ng/ul	2310130	4	16.87	1390510	20.0
unknown-04	17.25	71.9	ng/ul	4998850	4	16.87	1390510	20.0
7,9-Di-tert-butyl...	17.56	2.1	ng/ul	148608	4	16.87	1390510	20.0
Tridecanoic acid	17.80	2.3	ng/ul	162946	4	16.87	1390510	20.0
unknown-05	18.13	2.1	ng/ul	143197	4	16.87	1390510	20.0
unknown-06	18.52	2.8	ng/ul	197223	4	16.87	1390510	20.0
unknown-07	18.56	6.7	ng/ul	466512	4	16.87	1390510	20.0
Octadecanoic acid	19.09	4.3	ng/ul	406505	5	21.09	1878420	20.0
unknown-08	19.66	2.3	ng/ul	215880	5	21.09	1878420	20.0
Hexadecanoic acid...	19.70	5.3	ng/ul	499005	5	21.09	1878420	20.0
Myristin, 1,3-dia...	20.67	3.4	ng/ul	318109	5	21.09	1878420	20.0
Hexadecanoic acid...	21.51	2.2	ng/ul	205283	5	21.09	1878420	20.0
unknown-09	21.54	4.4	ng/ul	410300	5	21.09	1878420	20.0
Octadecanoic acid...	22.40	3.2	ng/ul	255965	6	23.23	1607120	20.0
unknown-10	22.43	5.7	ng/ul	461021	6	23.23	1607120	20.0