

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
 Data File : BM010613.D
 Acq On : 21 Jun 2017 05:06
 Operator : SJ/MA
 Sample : I3790-14
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C0B87

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	6.645	632	639	646	rVB	91252	144538	4.89%	0.372%
2	6.816	662	668	677	rVB	269361	391384	13.23%	1.006%
3	7.004	692	700	709	rBB	319215	483210	16.34%	1.242%
4	7.463	769	778	785	rBB	286796	444890	15.04%	1.144%
5	8.169	892	898	908	rBV2	272240	409122	13.83%	1.052%
6	8.551	958	963	967	rBV	35928	52072	1.76%	0.134%
7	8.610	967	973	981	rVB	387587	594596	20.11%	1.528%
8	9.322	1087	1094	1102	rBB	371677	578922	19.58%	1.488%
9	9.851	1177	1184	1193	rBV	531500	844096	28.54%	2.170%
10	10.145	1229	1234	1239	rVB4	17584	30770	1.04%	0.079%
11	10.227	1241	1248	1254	rBV	426891	666000	22.52%	1.712%
12	10.739	1330	1335	1342	rBV	24601	36631	1.24%	0.094%
13	13.027	1719	1724	1730	rVB	30791	41108	1.39%	0.106%
14	13.539	1804	1811	1817	rBV	1161935	1569002	53.05%	4.033%
15	13.804	1849	1856	1863	rBV	1159509	1641859	55.52%	4.220%
16	14.115	1903	1909	1917	rVB2	679646	1021807	34.55%	2.626%
17	14.321	1939	1944	1950	rVB	117892	161485	5.46%	0.415%
18	14.580	1980	1988	1997	rBV	358489	571129	19.31%	1.468%
19	15.121	2073	2080	2089	rVB	1496528	2112405	71.43%	5.430%
20	15.239	2095	2100	2106	rBV	565982	758982	25.66%	1.951%
21	16.309	2273	2282	2292	rBV	258177	348778	11.79%	0.896%
22	16.874	2371	2378	2384	rVB2	955903	1351256	45.69%	3.473%
23	16.974	2388	2395	2402	rVB	1758547	2484545	84.01%	6.386%
24	17.192	2427	2432	2436	rBV2	111424	126292	4.27%	0.325%
25	17.239	2436	2440	2450	rVB	221339	266053	9.00%	0.684%
26	17.562	2490	2495	2501	rVB2	190932	226833	7.67%	0.583%
27	17.809	2530	2537	2544	rBV	1198183	1686779	57.04%	4.336%
28	18.133	2585	2592	2598	rBV4	20151	30775	1.04%	0.079%
29	18.521	2653	2658	2661	rBV	213360	254100	8.59%	0.653%
30	18.562	2661	2665	2672	rVB	453175	510493	17.26%	1.312%
31	18.968	2731	2734	2748	rVB6	28878	50249	1.70%	0.129%
32	19.103	2751	2757	2765	rBV	1621108	2112546	71.43%	5.430%
33	19.280	2781	2787	2796	rVV	2266481	2957349	100.00%	7.602%
34	19.374	2796	2803	2810	rVB	226691	331628	11.21%	0.852%

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35	19.662	2847	2852	2855	rBV	1173586	1347044	45.55%	3.462%
36	19.697	2855	2858	2872	rVB	2256370	2415526	81.68%	6.209%
37	20.421	2979	2981	2986	rVB6	37500	37733	1.28%	0.097%
38	20.639	3014	3018	3021	rBV	353661	391887	13.25%	1.007%
39	20.674	3021	3024	3032	rVB	664095	678853	22.95%	1.745%
40	21.086	3088	3094	3099	rBV	1521440	1844684	62.38%	4.742%
41	21.262	3121	3124	3128	rBV5	18995	30068	1.02%	0.077%
42	21.509	3162	3166	3168	rBV	240037	271032	9.16%	0.697%
43	21.539	3168	3171	3177	rVB	471256	512324	17.32%	1.317%
44	22.097	3262	3266	3269	rBV	124259	149036	5.04%	0.383%
45	22.127	3269	3271	3277	rVB6	55092	66278	2.24%	0.170%
46	22.186	3277	3281	3283	rBV5	44050	52956	1.79%	0.136%
47	22.397	3312	3317	3319	rBV	268457	335613	11.35%	0.863%
48	22.433	3319	3323	3335	rVB	537771	729188	24.66%	1.874%
49	23.097	3429	3436	3442	rVB2	1696406	2929302	99.05%	7.529%
50	23.227	3451	3458	3465	rVB	885703	1596422	53.98%	4.103%
51	23.762	3546	3549	3555	rVB5	48682	77092	2.61%	0.198%
52	24.280	3632	3637	3642	rBV9	38570	75014	2.54%	0.193%
53	25.274	3804	3806	3815	rVB9	37833	72712	2.46%	0.187%

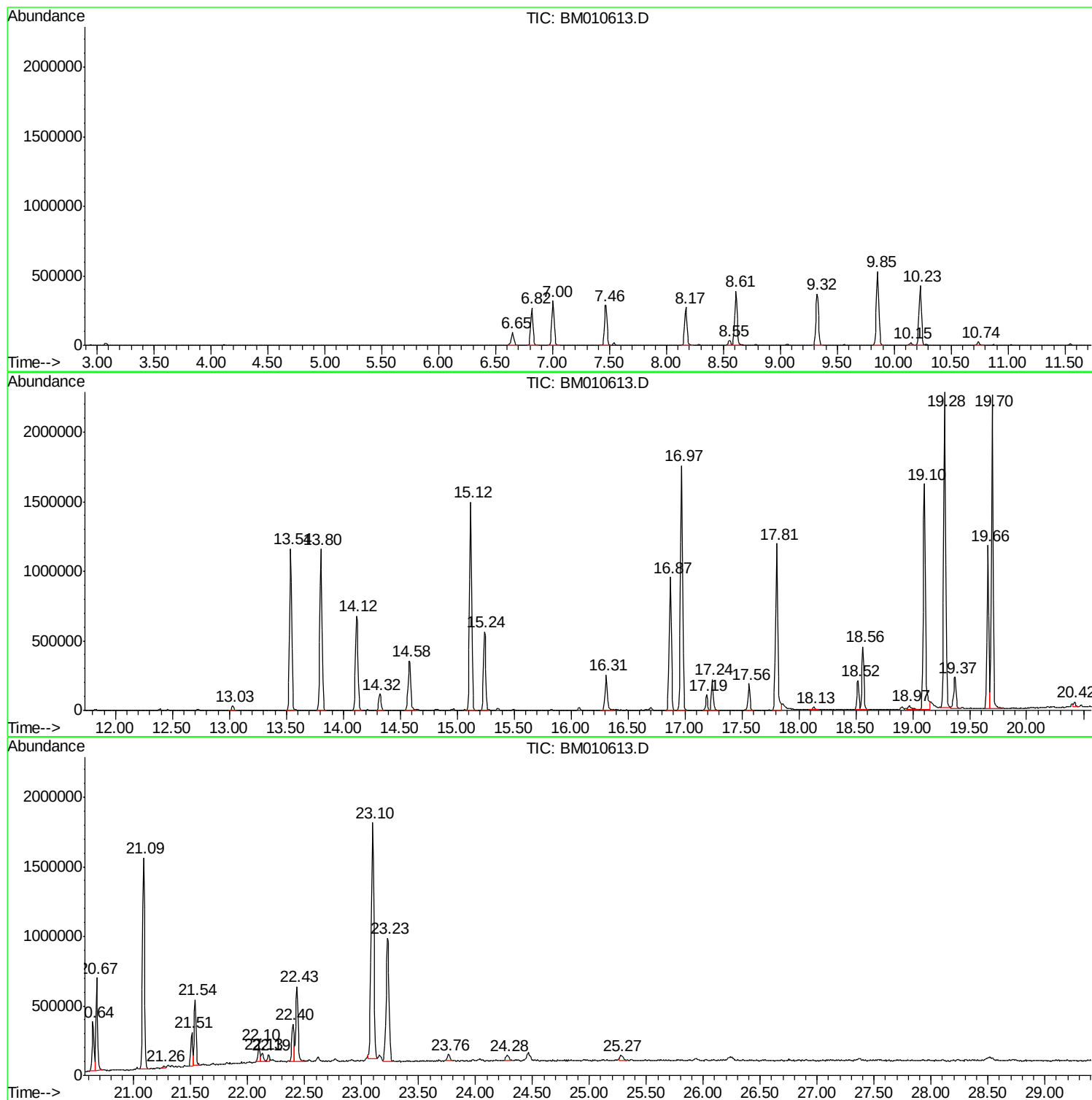
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Quant Title : SVOA CALIBRATION

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



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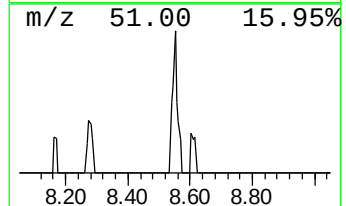
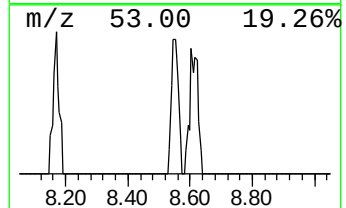
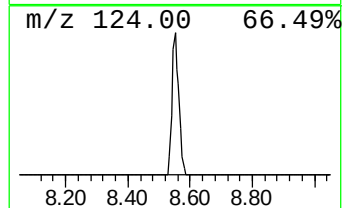
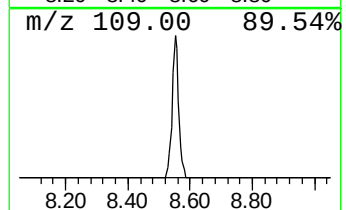
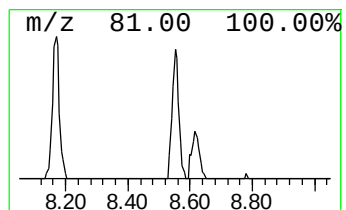
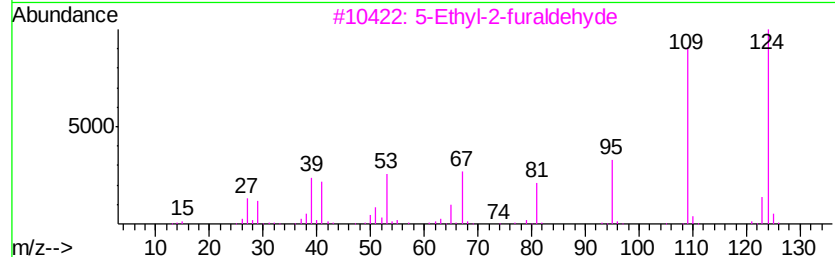
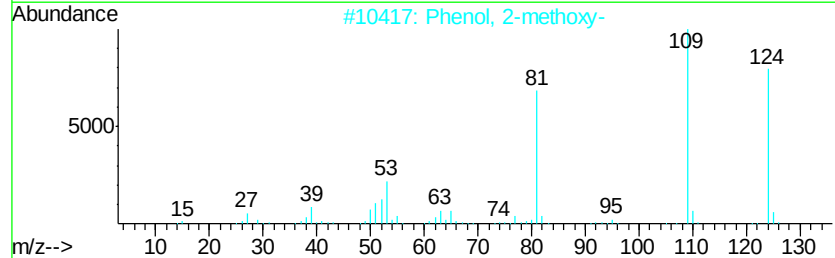
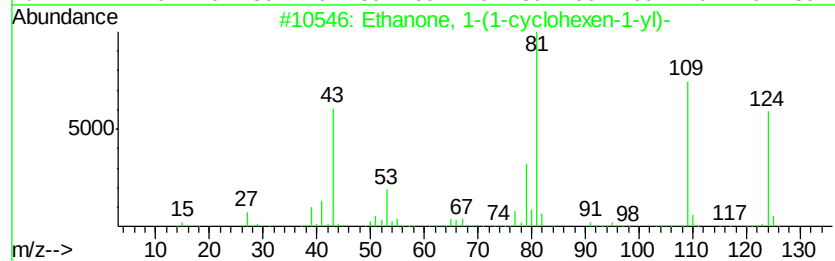
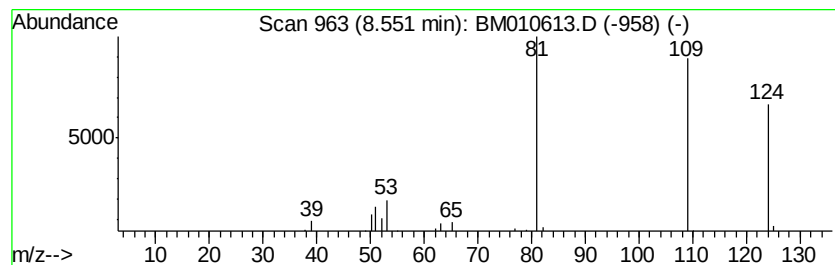
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 Ethanone, 1-(1-cyclohexen-1-yl) Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.55	2.34 ng/ul	52072	1,4-Dichlorobenzene-d4	7.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	80
2			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	52
3			5-Ethyl-2-furaldehyde	124	C7H8O2	023074-10-4	49
4			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	43
5			5-Ethyl-2-furaldehyde	124	C7H8O2	023074-10-4	43



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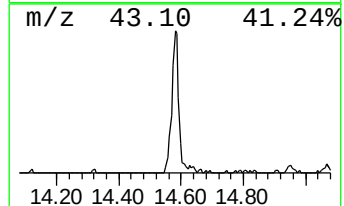
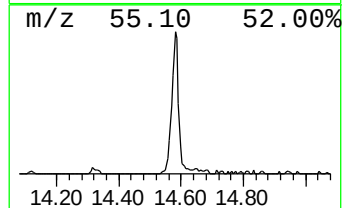
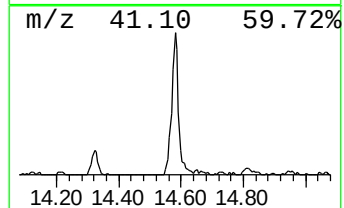
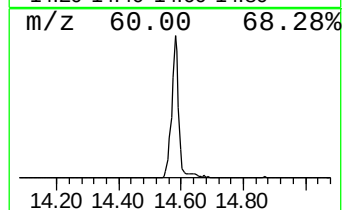
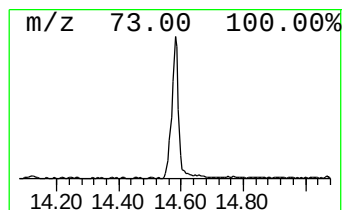
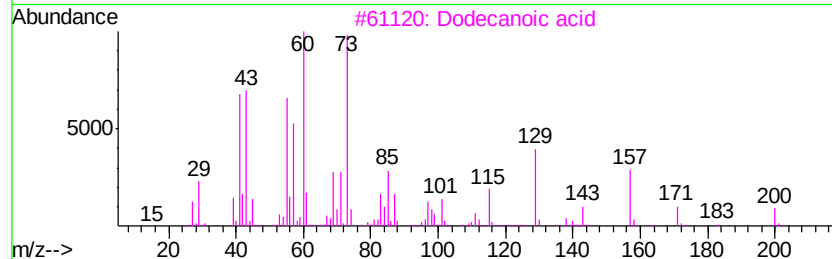
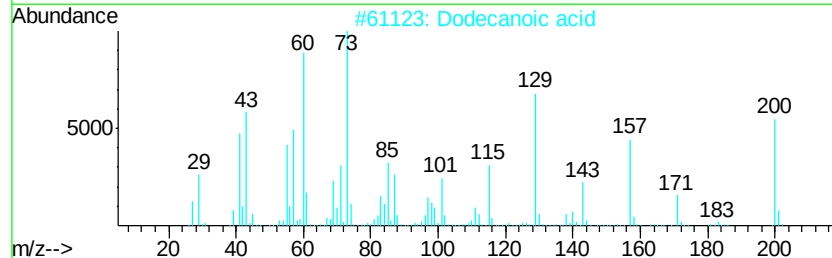
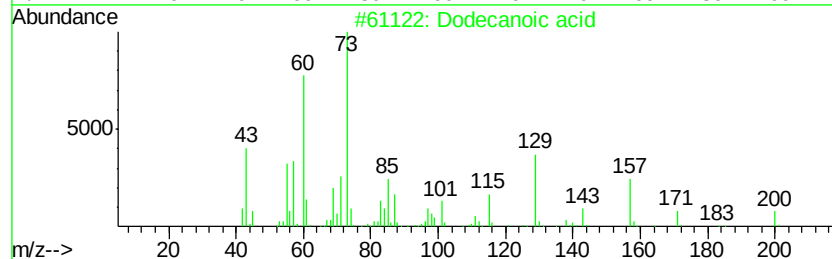
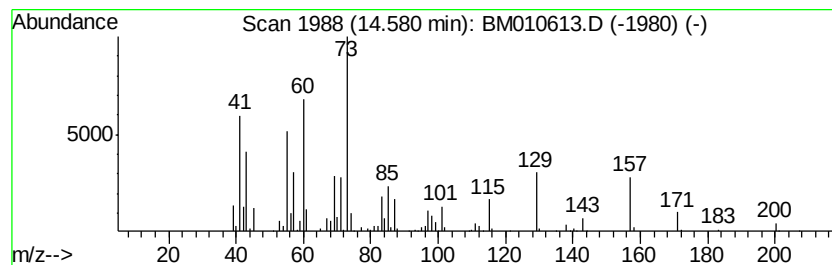
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	11.18 ng/ul	571129	Acenaphthene-d10	14.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	96
2		Dodecanoic acid	200	C12H24O2	000143-07-7	95
3		Dodecanoic acid	200	C12H24O2	000143-07-7	94
4		Dodecanoic acid	200	C12H24O2	000143-07-7	93
5		Dodecanoic acid	200	C12H24O2	000143-07-7	93



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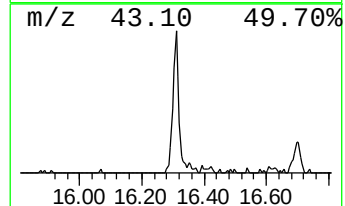
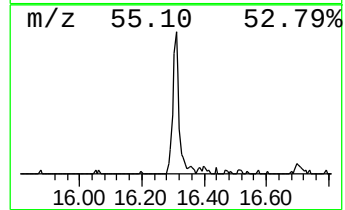
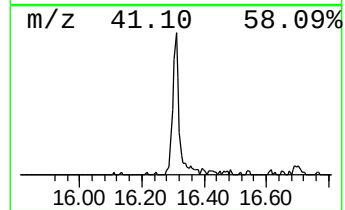
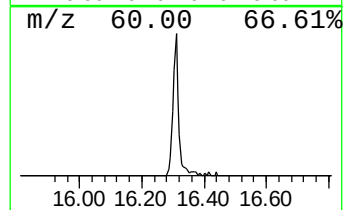
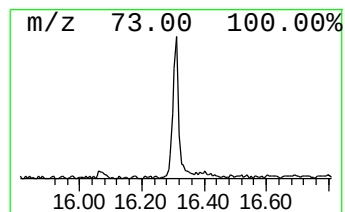
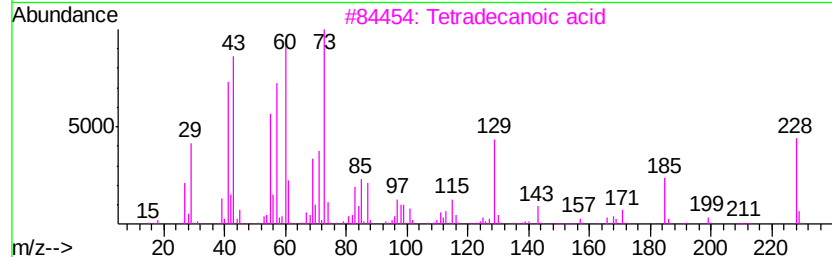
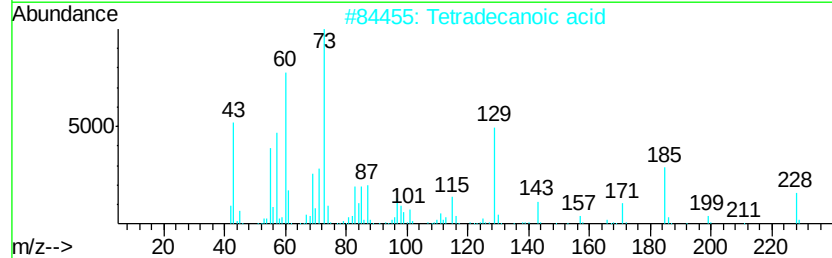
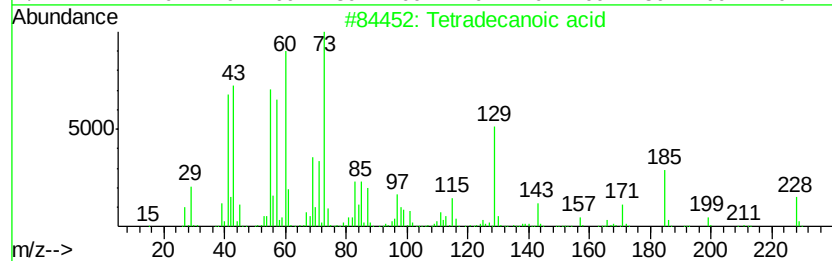
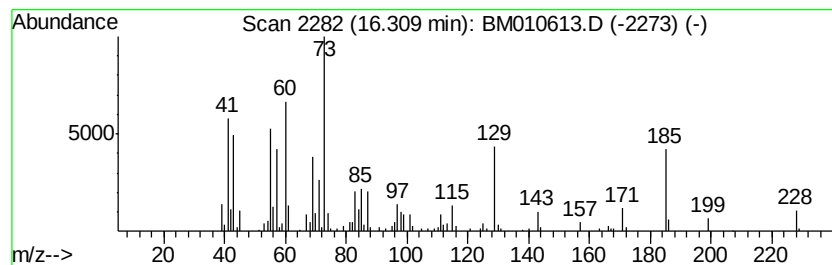
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Tetradecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	5.16 ng/ul	348778	Phenanthrene-d10	16.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	96
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	96
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	49



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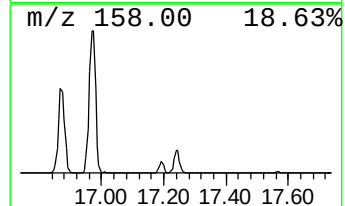
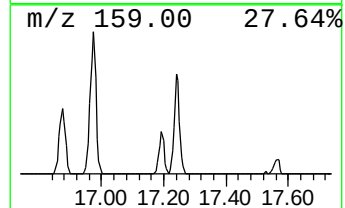
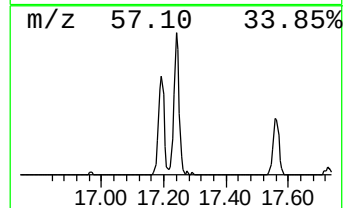
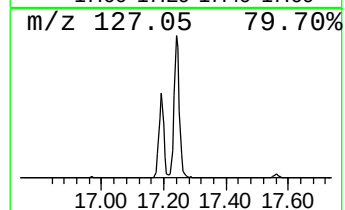
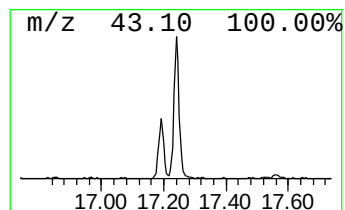
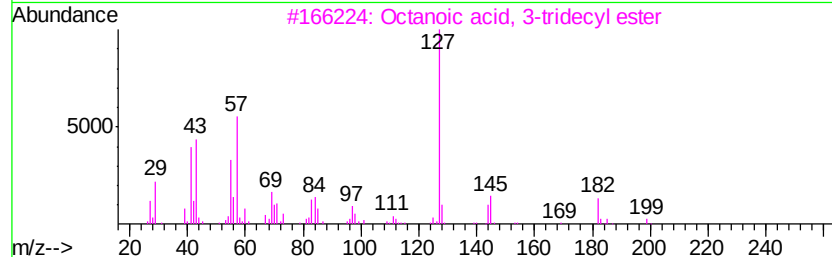
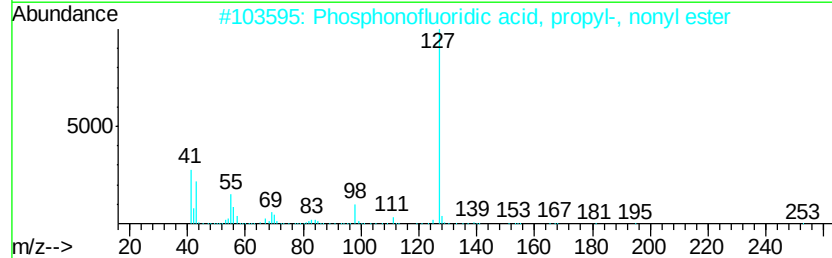
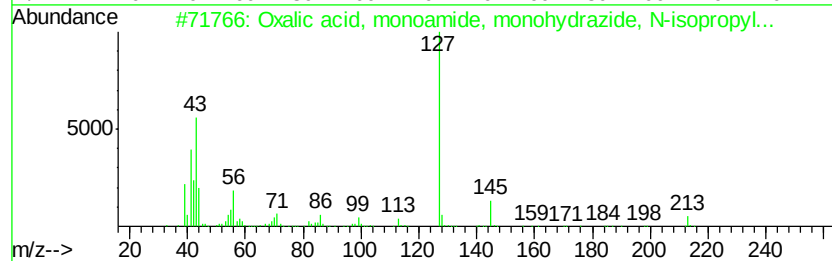
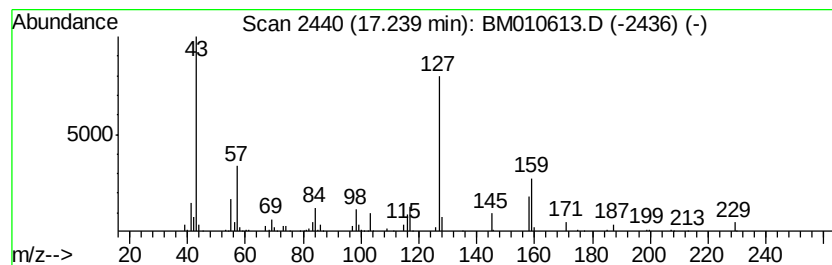
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Peak Number 4 unknown-01 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.24	3.94 ng/ul	266053	Phenanthrene-d10	16.87		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxalic acid, monoamide, monohydr...	213	C10H19N3O2	1000265-20-0	43
2		Phosphonofluoridic acid, propyl-...	252	C12H26F02P	333416-21-0	38
3		Octanoic acid, 3-tridecyl ester	326	C21H42O2	1000280-62-5	38
4		4-Amino-2,6-dihydroxypyrimidine	127	C4H5N3O2	000873-83-6	35
5		Propylphosphonic acid, fluoroanh...	238	C11H24F02P	1000273-50-7	32



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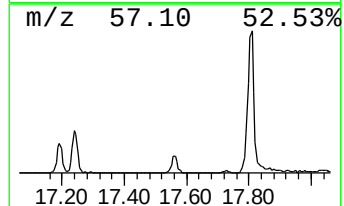
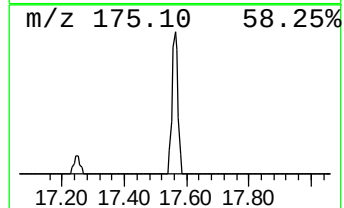
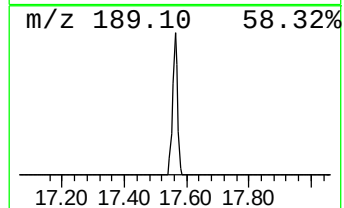
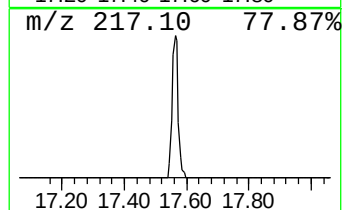
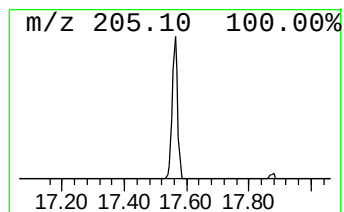
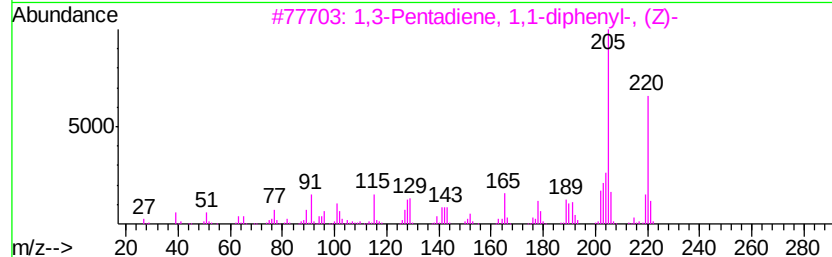
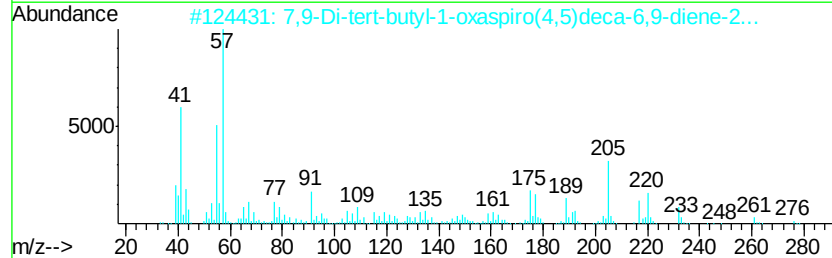
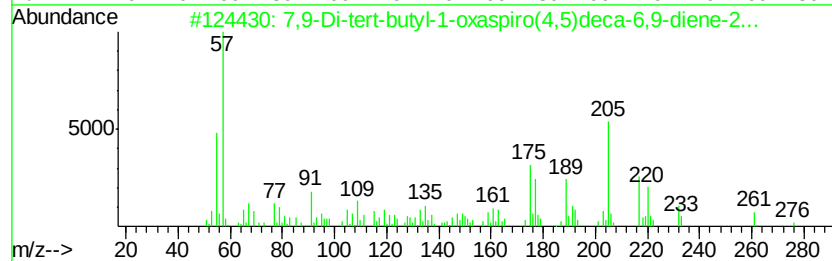
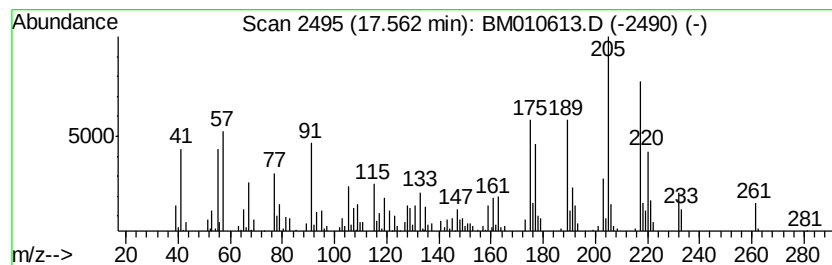
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.56	3.36 ng/ul	226833	Phenanthrene-d10	16.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	90
2		7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	64
3		1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	38
4		Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	38
5		1-Aminopyrene	217	C16H11N	001606-67-3	35



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010613.D
Acq On : 21 Jun 2017 05:06
Operator : SJ/MA
Sample : I3790-14
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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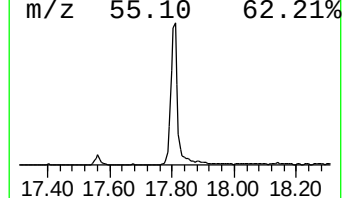
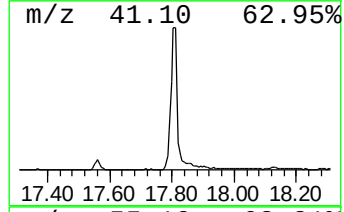
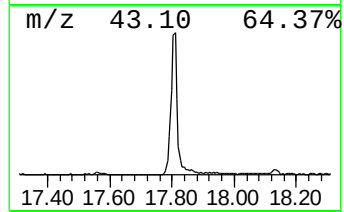
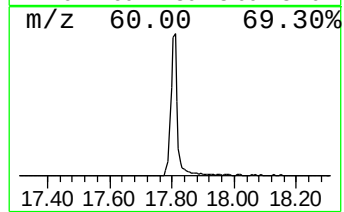
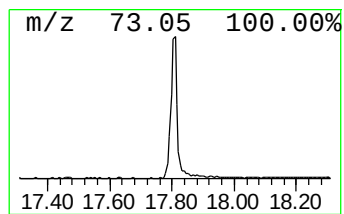
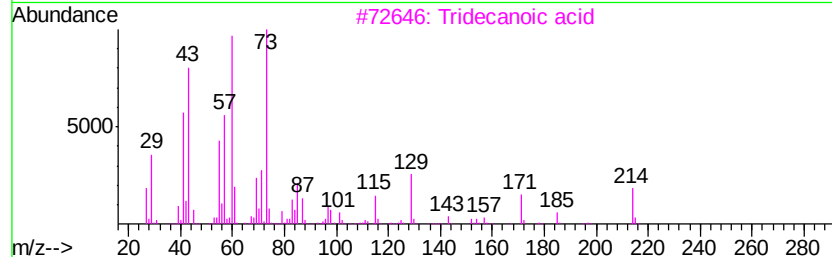
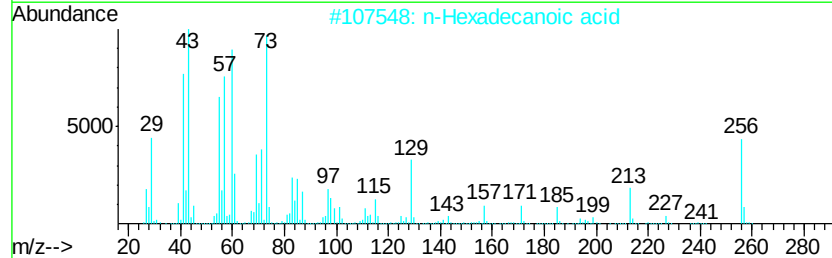
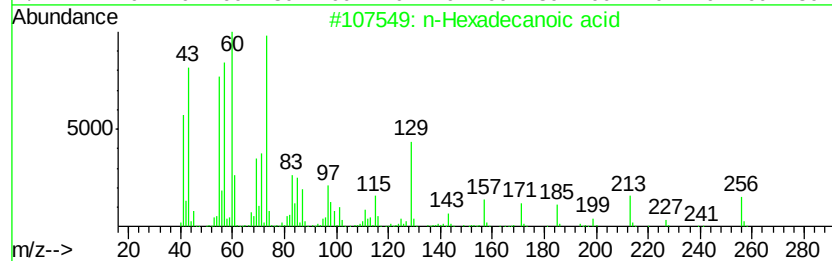
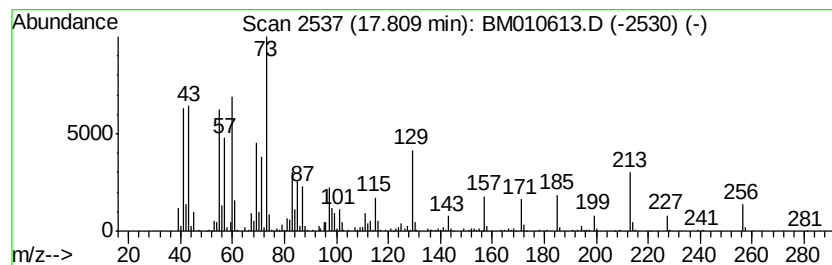
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.81	24.97 ng/ul	1686780	Phenanthrene-d10	16.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3		Tridecanoic acid	214	C13H26O2	000638-53-9	93
4		Tridecanoic acid	214	C13H26O2	000638-53-9	92
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	89



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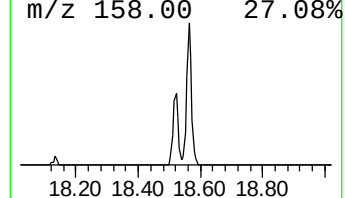
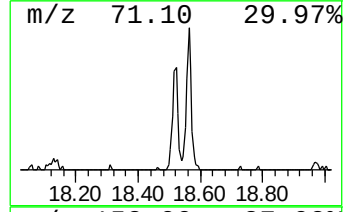
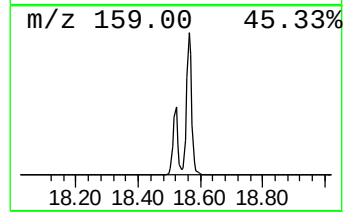
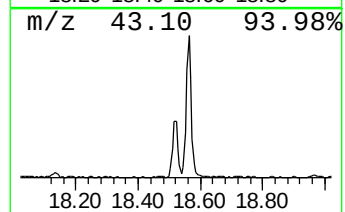
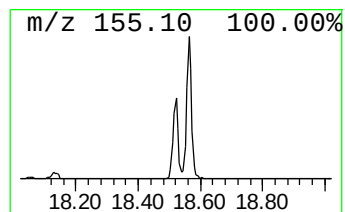
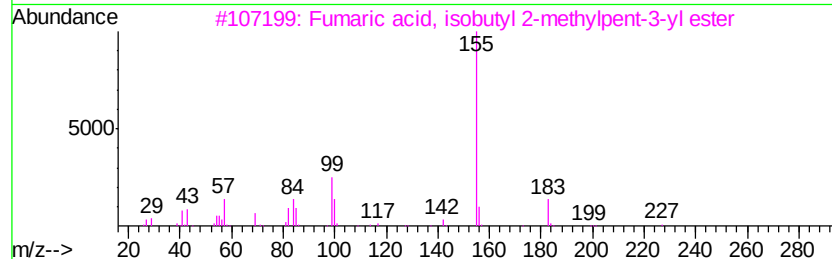
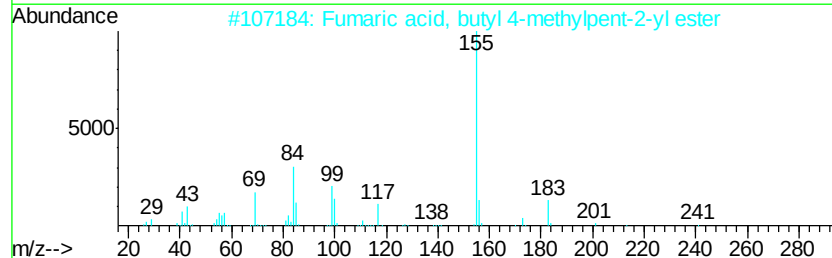
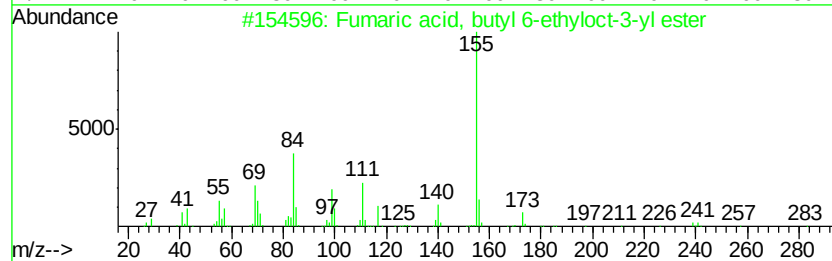
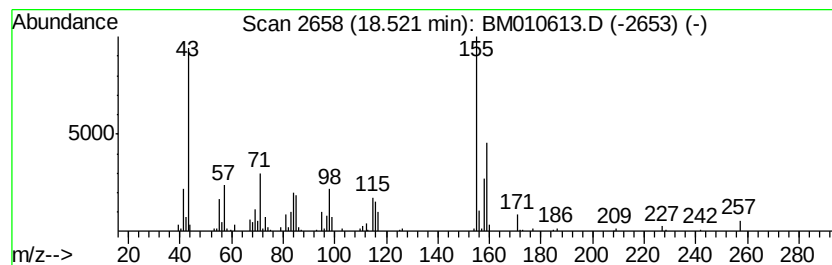
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-02 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.52	3.76 ng/ul	254100	Phenanthrene-d10	16.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fumaric acid, butyl 6-ethyloct-3...	312	C18H32O4	1000339-15-1	37
2		Fumaric acid, butyl 4-methylpent...	256	C14H24O4	1000348-31-7	37
3		Fumaric acid, isobutyl 2-methylp...	256	C14H24O4	1000348-76-0	32
4		Fumaric acid, butyl 3-hexyl ester	256	C14H24O4	1000348-60-4	32
5		Acetic acid, 2-[methyl(2,3,4,5-t...	200	C6H8N4O4	1000351-66-8	32



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010613.D
Acq On : 21 Jun 2017 05:06
Operator : SJ/MA
Sample : I3790-14
Misc :
ALS Vial : 24 Sample Multiplier: 1

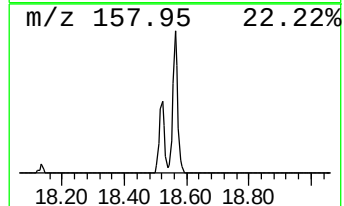
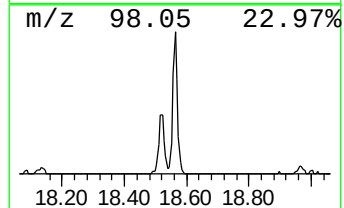
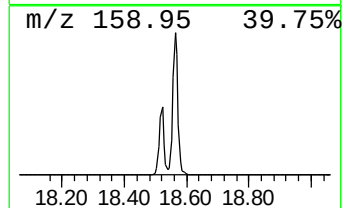
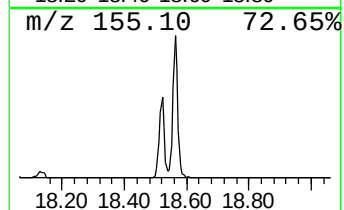
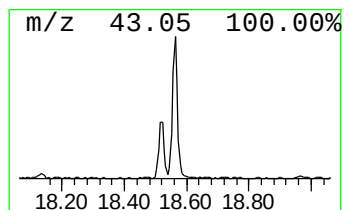
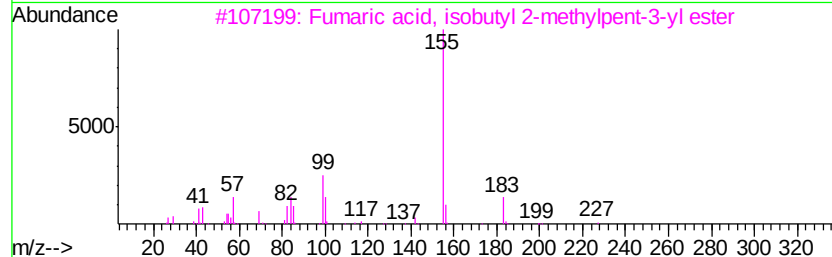
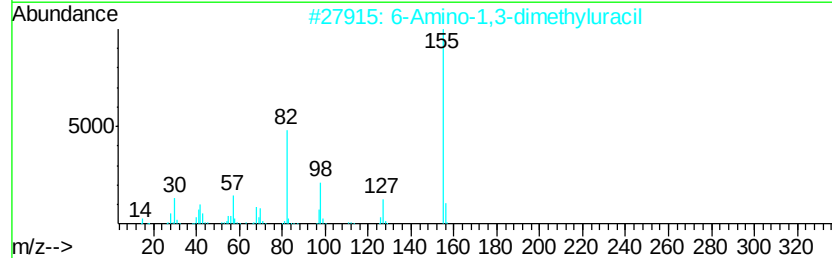
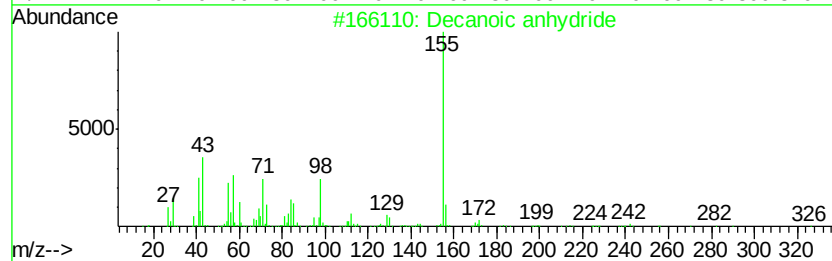
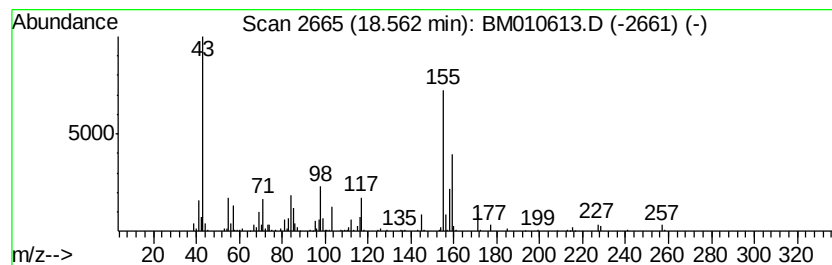
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 unknown-03 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.56	7.56 ng/ul	510493	Phenanthrene-d10		16.87
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic anhydride	326	C20H38O3	002082-76-0	27
2	6-Amino-1,3-dimethyluracil	155	C6H9N3O2	006642-31-5	22
3	Fumaric acid, isobutyl 2-methylp...	256	C14H24O4	1000348-76-0	22
4	Decanoic anhydride	326	C20H38O3	002082-76-0	22
5	Fumaric acid, 2-hexyl isobutyl e...	256	C14H24O4	1000348-74-1	16



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010613.D
Acq On : 21 Jun 2017 05:06
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Sample : I3790-14
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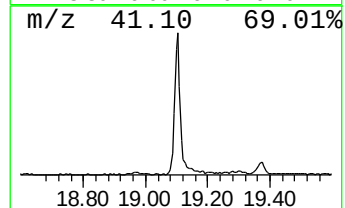
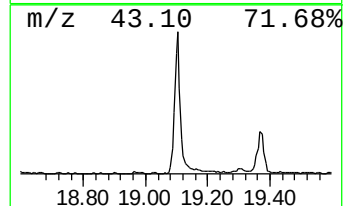
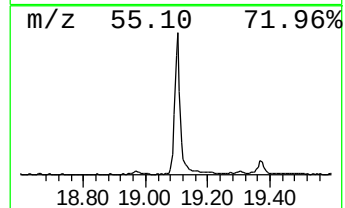
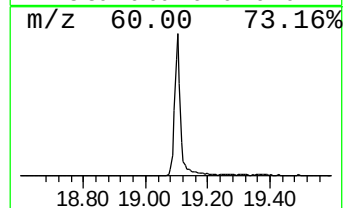
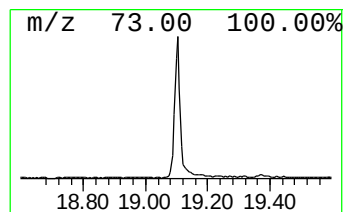
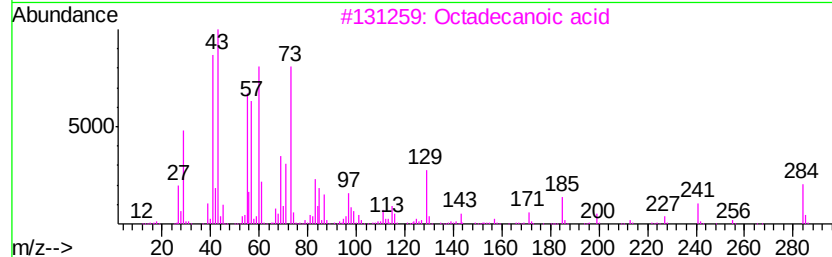
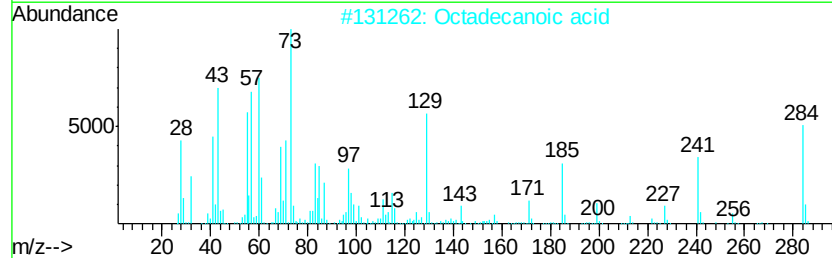
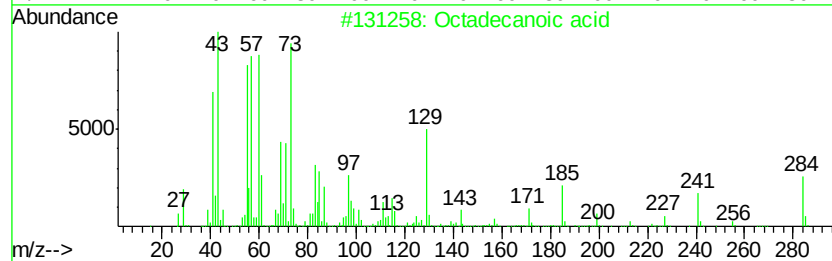
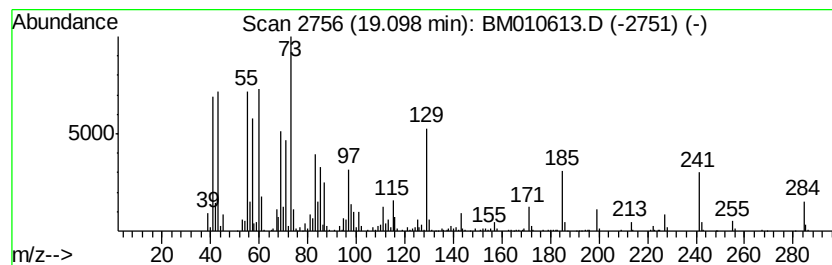
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.10	22.90 ng/ul	2112550	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	98
3		Octadecanoic acid	284	C18H36O2	000057-11-4	96
4		Octadecanoic acid	284	C18H36O2	000057-11-4	93
5		Octadecanoic acid	284	C18H36O2	000057-11-4	90



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
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Acq On : 21 Jun 2017 05:06
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Misc :
ALS Vial : 24 Sample Multiplier: 1

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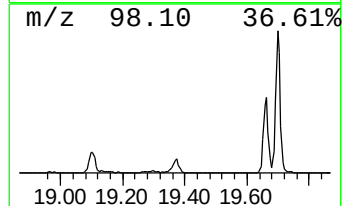
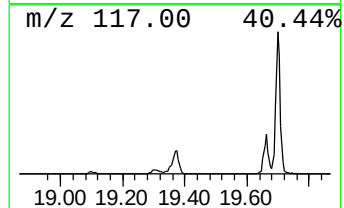
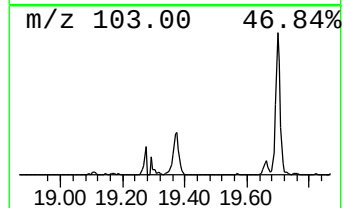
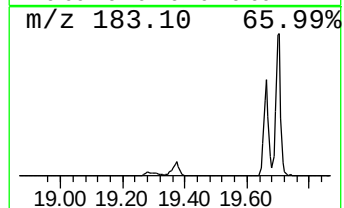
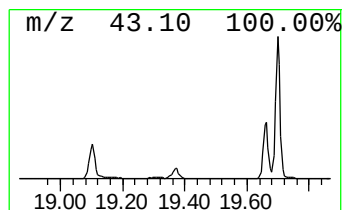
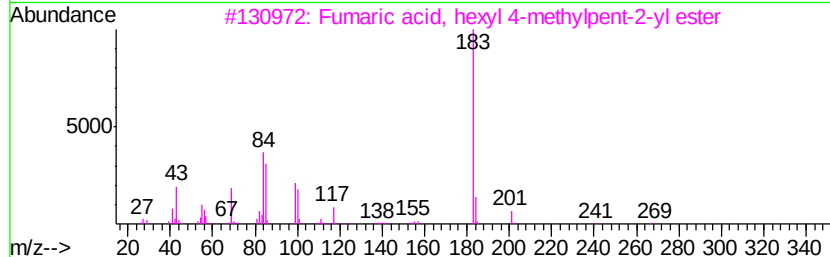
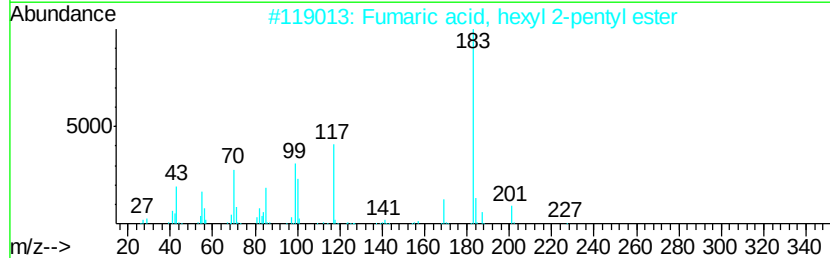
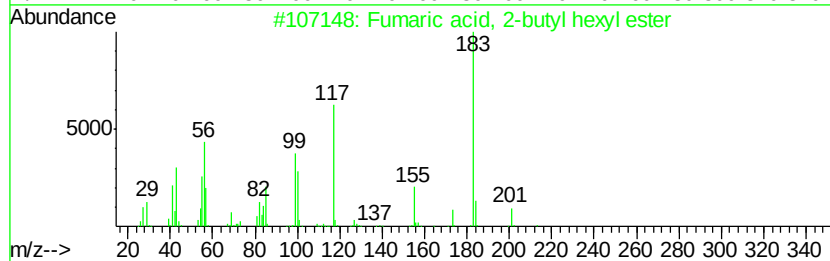
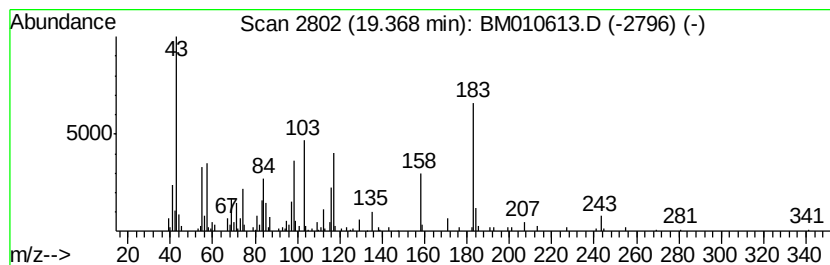
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 unknown-04 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.37	3.60 ng/ul	331628	Chrysene-d12	21.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fumaric acid, 2-butyl hexyl ester	256	C14H24O4	1000348-64-3	25
2			Fumaric acid, hexyl 2-pentyl ester	270	C15H26O4	1000330-41-6	25
3			Fumaric acid, hexyl 4-methylpent...	284	C16H28O4	1000348-32-0	16
4			Lauric anhydride	382	C24H46O3	000645-66-9	16
5			Dodecanoic acid, 2,4,5-trichloro...	378	C18H25Cl3O2	1000360-54-9	14



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
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Sample : I3790-14
Misc :
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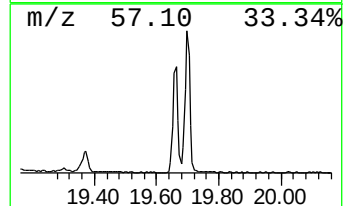
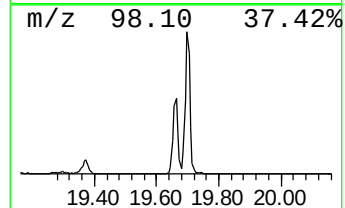
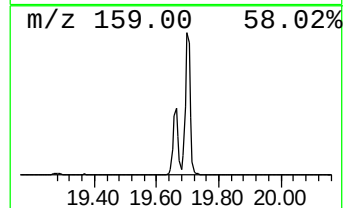
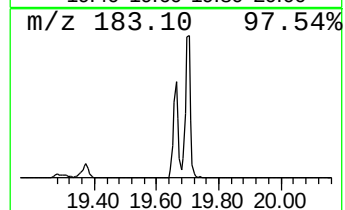
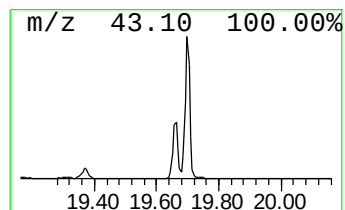
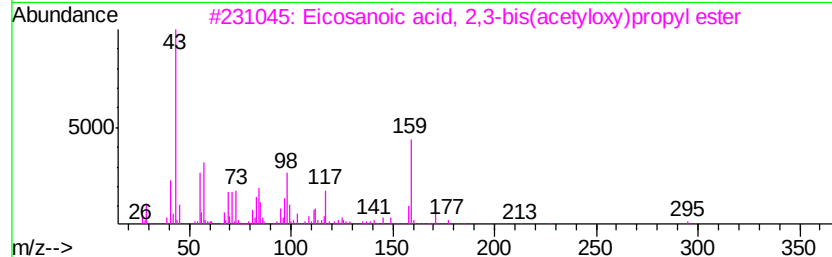
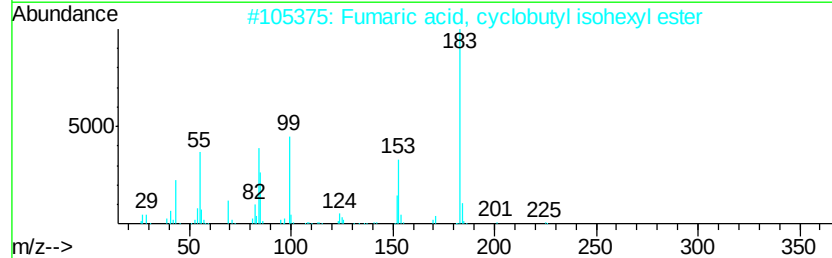
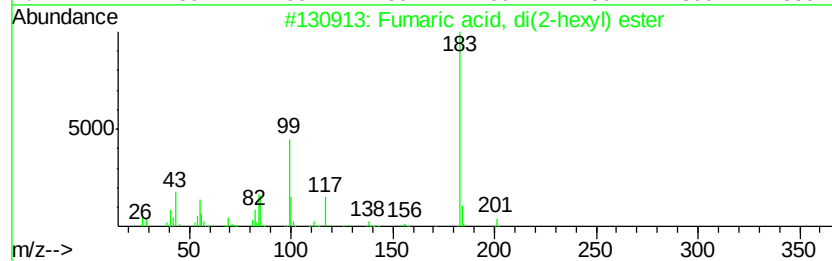
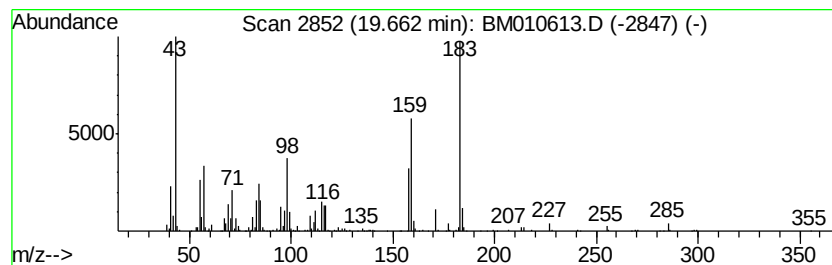
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 unknown-05 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.66	14.60 ng/ul	1347040	Chrysene-d12	21.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fumaric acid, di(2-hexyl) ester	284	C16H28O4	1000348-75-8	35
2		Fumaric acid, cyclobutyl isohexy...	254	C14H22O4	1000345-03-5	35
3		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	32
4		Dodecanoic acid, 2,4,5-trichloro...	378	C18H25Cl3O2	1000360-54-9	30
5		4-Methoxy-3-nitrobenzyl alcohol	183	C8H9NO4	041870-24-0	27



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010613.D
Acq On : 21 Jun 2017 05:06
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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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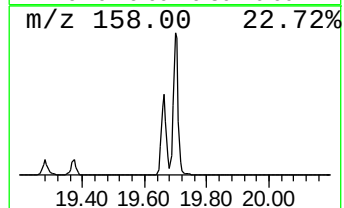
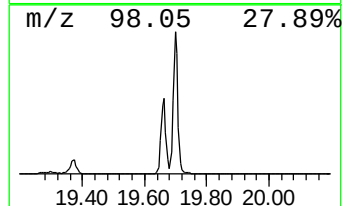
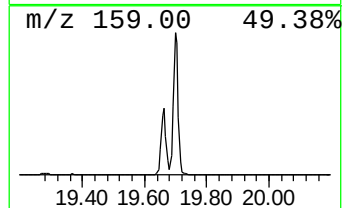
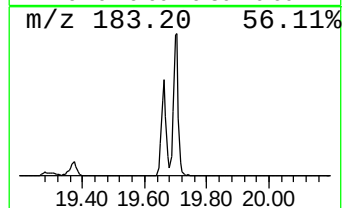
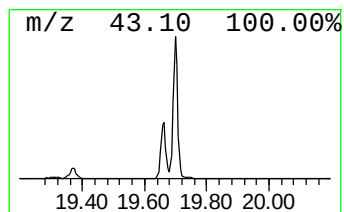
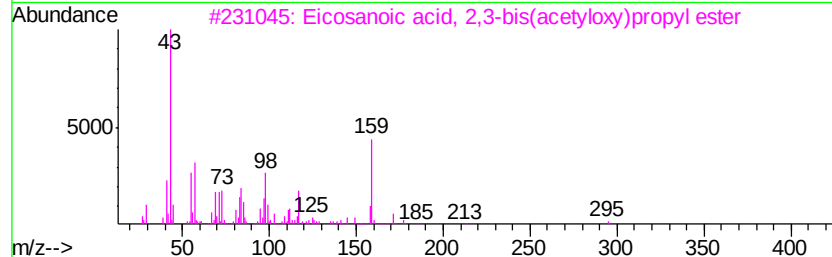
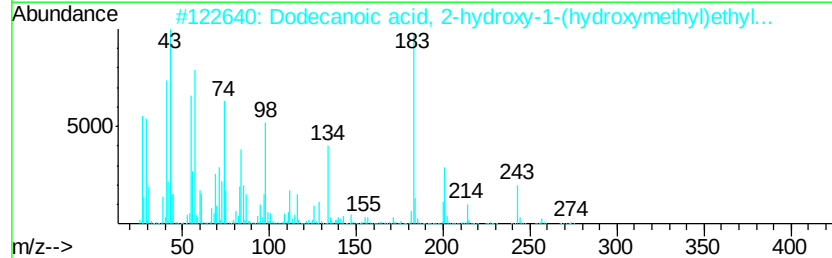
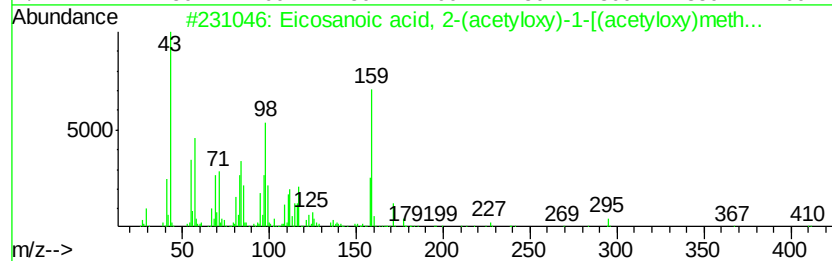
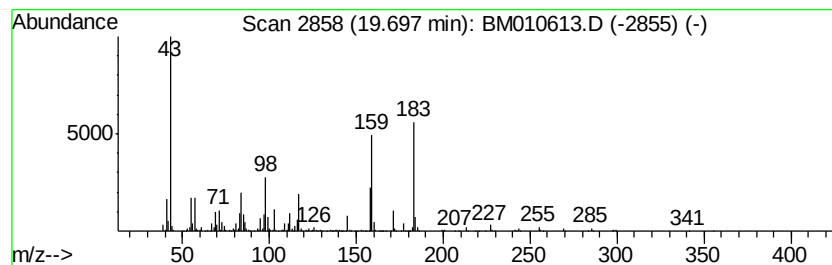
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Quant Title : SVOA CALIBRATION

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

Peak Number 12 unknown-06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.70	26.19 ng/ul	2415530	Chrysene-d12	21.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	40
2		Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	38
3		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	37
4		Lauric anhydride	382	C24H46O3	000645-66-9	22
5		Fumaric acid, cyclobutyl isohexy...	254	C14H22O4	1000345-03-5	22



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010613.D
Acq On : 21 Jun 2017 05:06
Operator : SJ/MA
Sample : I3790-14
Misc :
ALS Vial : 24 Sample Multiplier: 1

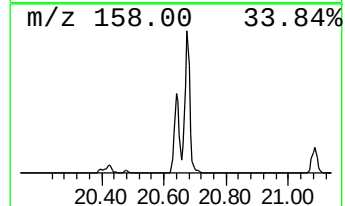
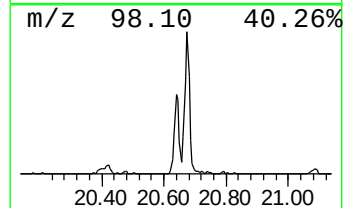
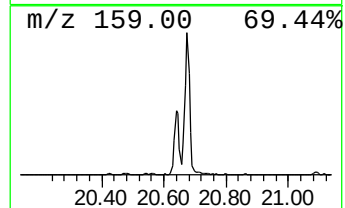
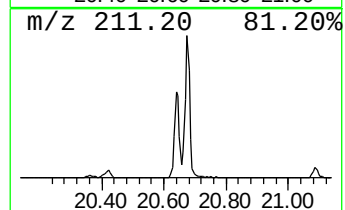
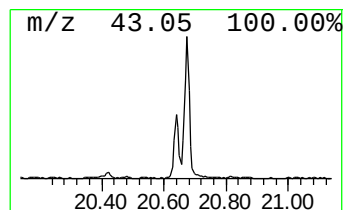
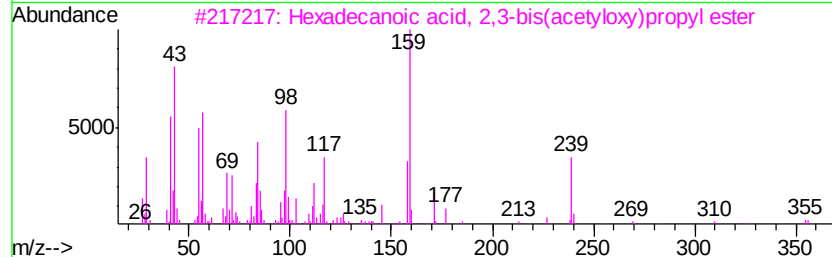
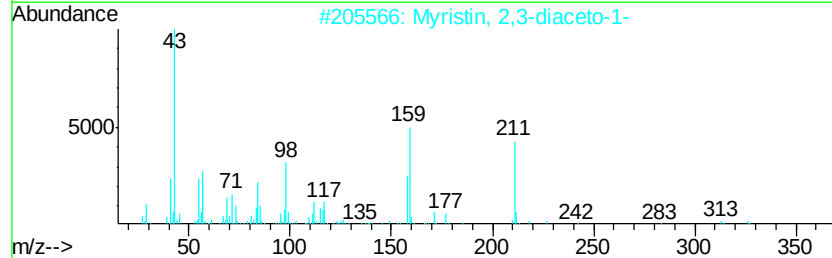
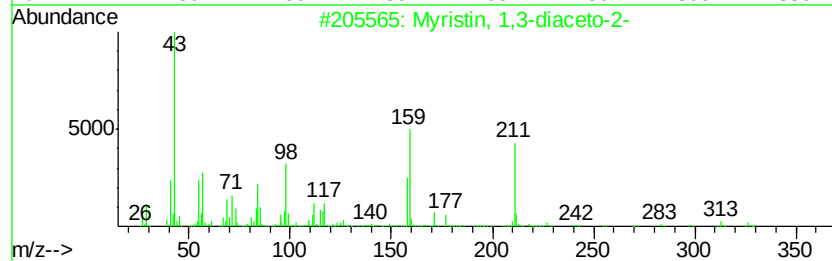
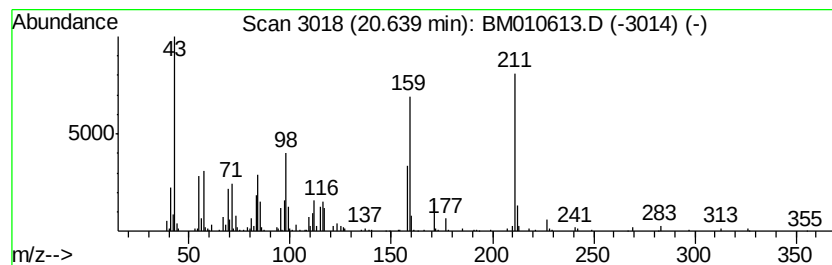
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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

Peak Number 13 Myristin, 1,3-diaceto-2- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
20.64	4.25 ng/ul	391887	Chrysene-d12	21.09		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin,	1,3-diaceto-2-	386	C21H38O6	014290-23-4	81
2	Myristin,	2,3-diaceto-1-	386	C21H38O6	014473-55-3	81
3	Hexadecanoic acid,	2,3-bis(acety...	414	C23H42O6	055268-70-7	53
4	1,1,7,7-Tetramethyl-4-vinyl-1,4,...		332	C10H23Cl3Si3	102105-66-8	27
5	Fumaric acid,	2-decyl octyl ester	368	C22H40O4	1000348-59-0	25



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010613.D
Acq On : 21 Jun 2017 05:06
Operator : SJ/MA
Sample : I3790-14
Misc :
ALS Vial : 24 Sample Multiplier: 1

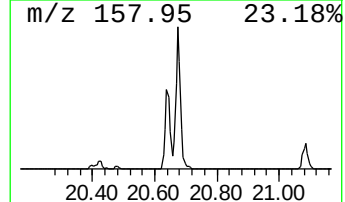
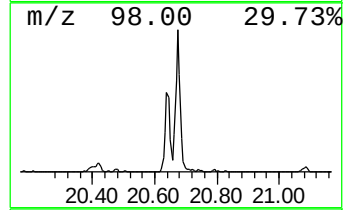
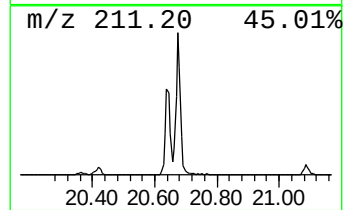
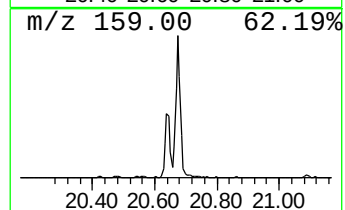
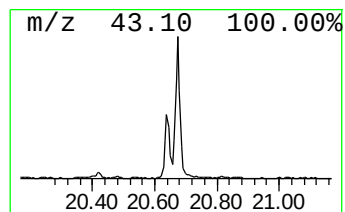
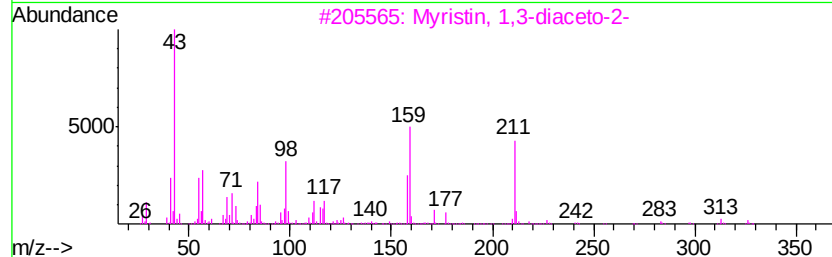
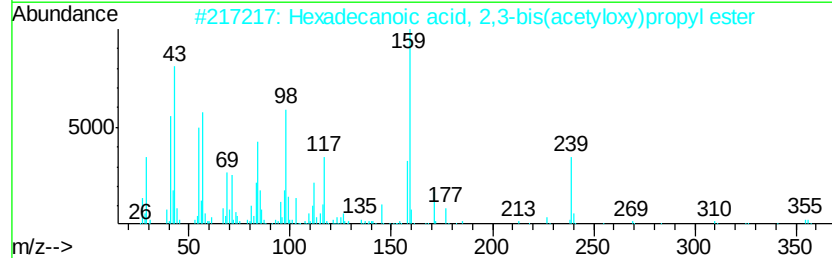
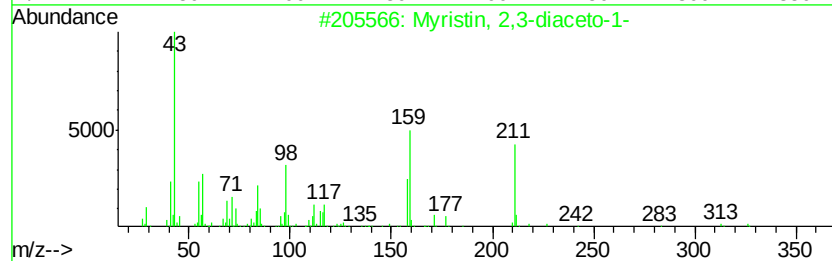
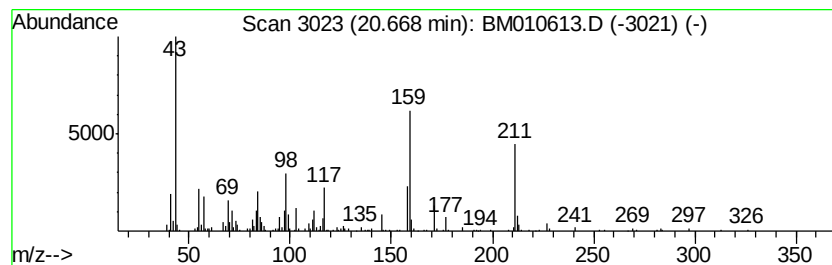
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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

Peak Number 14 Myristin, 2,3-diaceto-1- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
20.67	7.36 ng/ul	678853	Chrysene-d12	21.09		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	83	
2	Hexadecanoic acid, 2,3-bis(acetyloxy)propyl ester	414	C23H42O6	055268-70-7	70	
3	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	68	
4	Pyridine, 1,2,3,6-tetrahydro-4-pyridyl ester	159	C11H13N	010338-69-9	14	
5	Nonanoic acid, dodecyl ester	326	C21H42O2	1000340-27-9	11	



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010613.D
Acq On : 21 Jun 2017 05:06
Operator : SJ/MA
Sample : I3790-14
Misc :
ALS Vial : 24 Sample Multiplier: 1

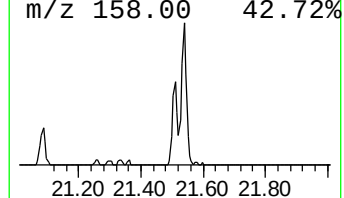
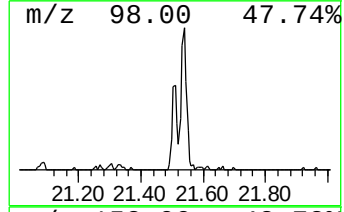
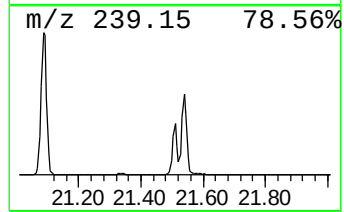
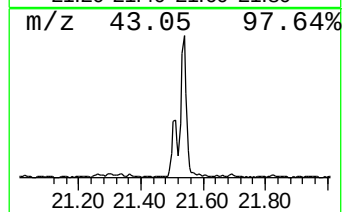
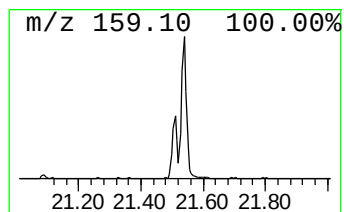
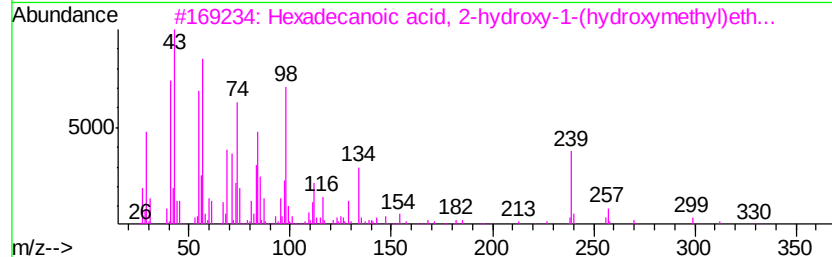
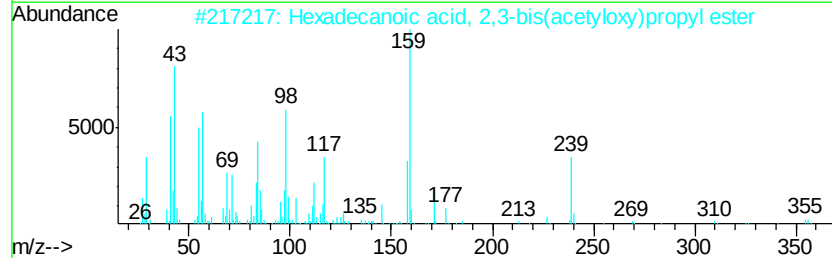
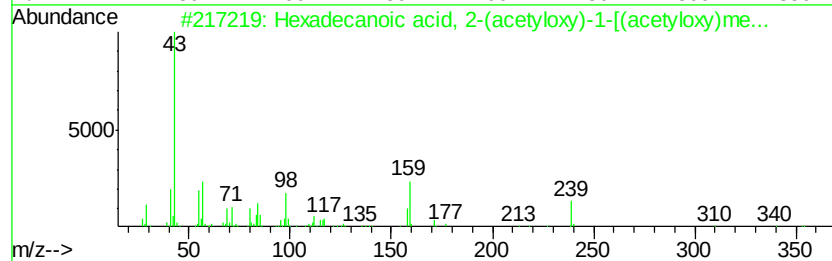
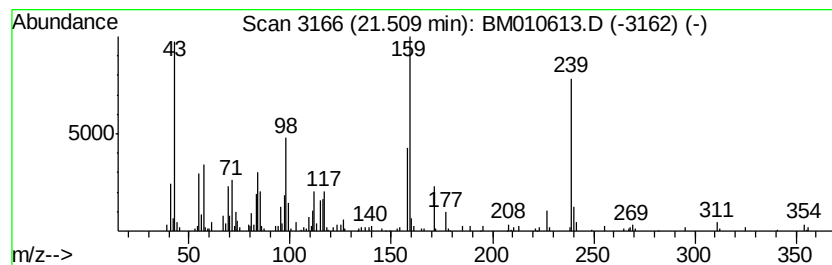
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM062017.M
Quant Title : SVOA CALIBRATION

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

Peak Number 15 Hexadecanoic acid, 2-(acety... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.51	2.94 ng/ul	271032	Chrysene-d12	21.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecanoic acid, 2-(acetyloxy)...	414 C23H42O6	055268-69-4	87
2	Hexadecanoic acid, 2,3-bis(acety...	414 C23H42O6	055268-70-7	87
3	Hexadecanoic acid, 2-hydroxy-1-(...	330 C19H38O4	023470-00-0	38
4	Eicosanoic acid, 2-(acetyloxy)-1...	470 C27H50O6	055429-68-0	27
5	1-Methyl-2-formylindole	159 C10H9NO	027421-51-8	22



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010613.D
Acq On : 21 Jun 2017 05:06
Operator : SJ/MA
Sample : I3790-14
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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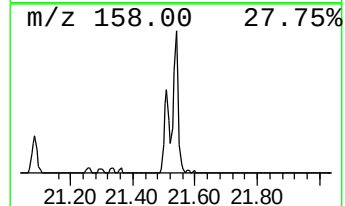
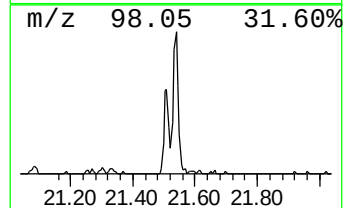
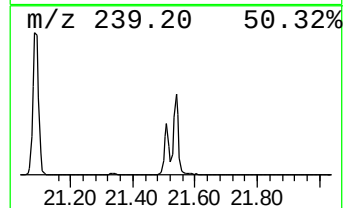
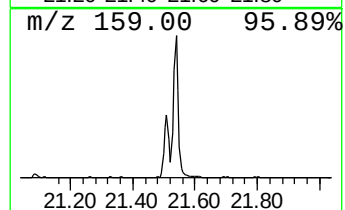
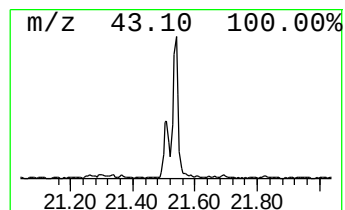
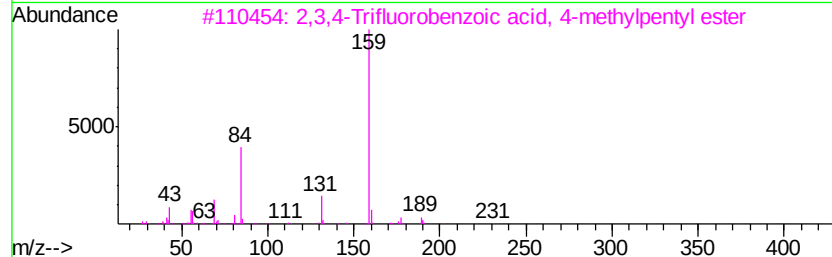
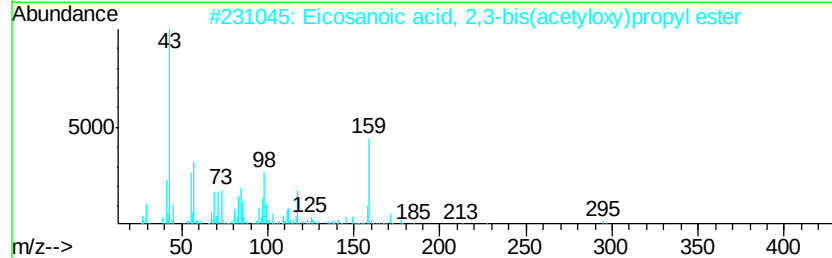
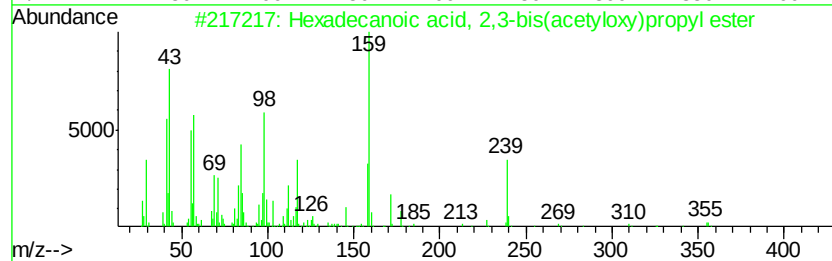
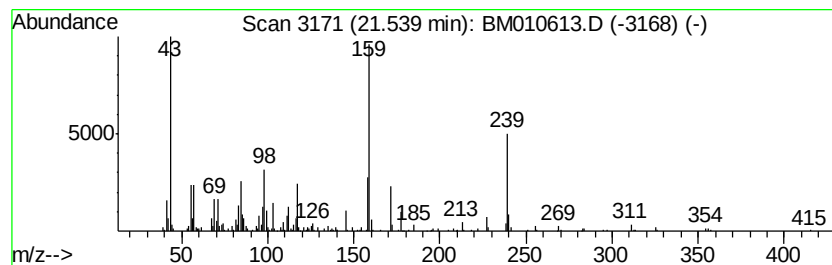
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Quant Title : SVOA CALIBRATION

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

Peak Number 16 Hexadecanoic acid, 2,3-bis(...) Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.54	5.55 ng/ul	512324	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	90
2		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	47
3		2,3,4-Trifluorobenzoic acid, 4-m...	260	C13H15F3O2	1000282-29-8	27
4		2,3,4-Trifluorobenzoic acid, 6-e...	316	C17H23F3O2	1000282-58-3	27
5		2,3,4-Trifluorobenzoic acid, 3-t...	358	C20H29F3O2	1000280-61-8	27



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
Data File : BM010613.D
Acq On : 21 Jun 2017 05:06
Operator : SJ/MA
Sample : I3790-14
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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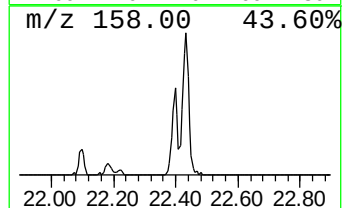
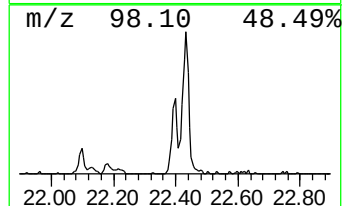
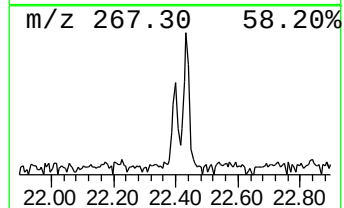
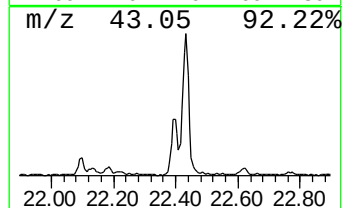
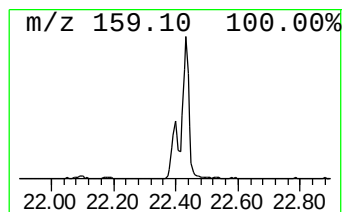
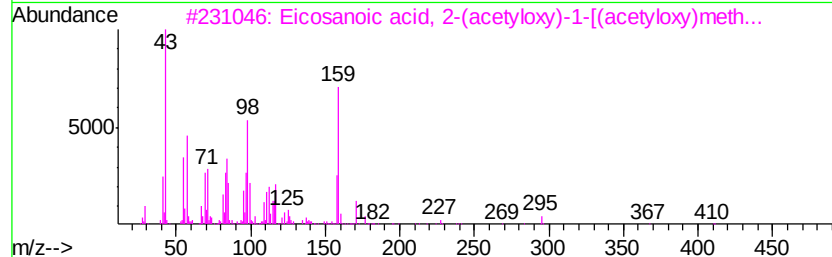
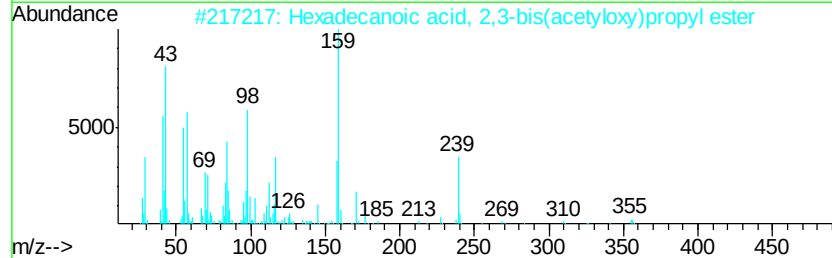
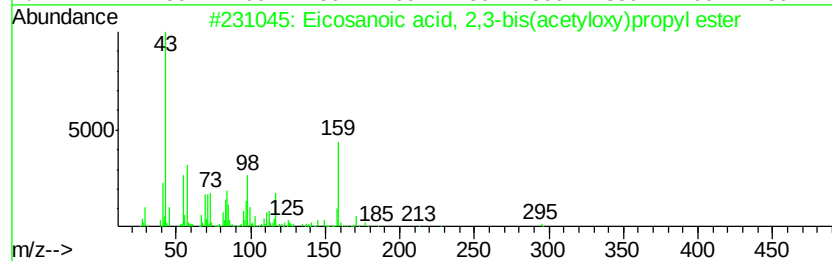
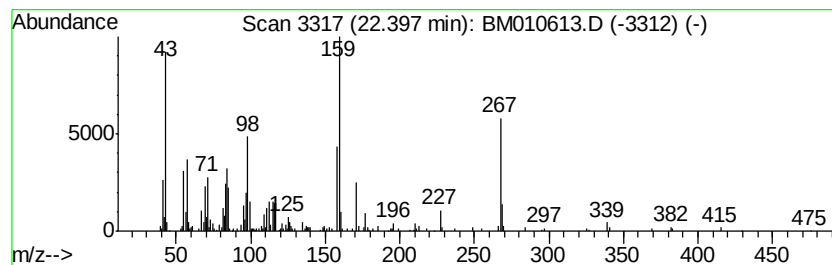
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Quant Title : SVOA CALIBRATION

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

Peak Number 17 Eicosanoic acid, 2,3-bis(ac... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.40	4.20 ng/ul	335613	Perylene-d12	23.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	50
2		Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	50
3		Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	45
4		Nonanoic acid, tridecyl ester	340	C22H44O2	1000340-28-0	35
5		2,3,4-Trifluorobenzoic acid, 4-p...	386	C22H33F3O2	1000280-62-3	27



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM062017\
 Data File : BM010613.D
 Acq On : 21 Jun 2017 05:06
 Operator : SJ/MA
 Sample : I3790-14
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
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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
Ethanone, 1-(1-cy...	8.55	2.3	ng/ul	52072	1	7.47	444890	20.0
Dodecanoic acid	14.58	11.2	ng/ul	571129	3	14.12	1021810	20.0
Tetradecanoic acid	16.31	5.2	ng/ul	348778	4	16.87	1351260	20.0
unknown-01	17.24	3.9	ng/ul	266053	4	16.87	1351260	20.0
7,9-Di-tert-butyl...	17.56	3.4	ng/ul	226833	4	16.87	1351260	20.0
n-Hexadecanoic acid	17.81	25.0	ng/ul	1686780	4	16.87	1351260	20.0
unknown-02	18.52	3.8	ng/ul	254100	4	16.87	1351260	20.0
unknown-03	18.56	7.6	ng/ul	510493	4	16.87	1351260	20.0
Octadecanoic acid	19.10	22.9	ng/ul	2112550	5	21.09	1844680	20.0
unknown-04	19.37	3.6	ng/ul	331628	5	21.09	1844680	20.0
unknown-05	19.66	14.6	ng/ul	1347040	5	21.09	1844680	20.0
unknown-06	19.70	26.2	ng/ul	2415530	5	21.09	1844680	20.0
Myristin, 1,3-dia...	20.64	4.3	ng/ul	391887	5	21.09	1844680	20.0
Myristin, 2,3-dia...	20.67	7.4	ng/ul	678853	5	21.09	1844680	20.0
Hexadecanoic acid...	21.51	2.9	ng/ul	271032	5	21.09	1844680	20.0
Hexadecanoic acid...	21.54	5.5	ng/ul	512324	5	21.09	1844680	20.0
Eicosanoic acid, ...	22.40	4.2	ng/ul	335613	6	23.23	1596420	20.0