

Data Path : Z:\HPCHEM1\BNA M\DATA\BM043017\
 Data File : BM009814.D
 Acq On : 30 Apr 2017 16:33
 Operator : SJ/MA
 Sample : I2849-19
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 JHSY3

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-BM042517.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	6.981	653	662	677	rBV	494357	906504	24.47%	1.876%
2	7.146	685	690	699	rVB	382133	577754	15.60%	1.196%
3	7.340	717	723	731	rBV	466489	755501	20.39%	1.563%
4	7.810	796	803	814	rBV	673972	1065819	28.77%	2.206%
5	8.516	916	923	931	rBV	535881	832636	22.47%	1.723%
6	8.981	995	1002	1011	rBV	481379	825634	22.29%	1.709%
7	9.698	1116	1124	1134	rBV	407254	683873	18.46%	1.415%
8	10.228	1206	1214	1226	rBV	569000	991055	26.75%	2.051%
9	10.610	1271	1279	1285	rBV	926739	1588662	42.88%	3.288%
10	10.757	1296	1304	1317	rBV	302699	573029	15.47%	1.186%
11	13.710	1798	1806	1811	rBV7	53572	86159	2.33%	0.178%
12	13.869	1822	1833	1837	rBV	1131095	1574660	42.50%	3.259%
13	13.916	1837	1841	1849	rVB	271695	376072	10.15%	0.778%
14	14.151	1874	1881	1888	rBV	1205378	1815206	49.00%	3.756%
15	14.327	1901	1911	1920	rVB2	115528	257047	6.94%	0.532%
16	14.463	1927	1934	1940	rBV2	1385126	2202987	59.46%	4.559%
17	14.527	1940	1945	1950	rVB6	31910	57372	1.55%	0.119%
18	14.680	1963	1971	1980	rBV	229796	448769	12.11%	0.929%
19	15.280	2070	2073	2078	rBV	70359	91004	2.46%	0.188%
20	15.451	2096	2102	2112	rVB	1577259	2357296	63.63%	4.878%
21	15.586	2119	2125	2133	rBV	427694	625774	16.89%	1.295%
22	15.692	2137	2143	2147	rVB6	43597	75258	2.03%	0.156%
23	15.910	2175	2180	2189	rVB9	17951	41247	1.11%	0.085%
24	16.145	2216	2220	2228	rBV	100735	179790	4.85%	0.372%
25	16.427	2262	2268	2272	rBV5	66473	94143	2.54%	0.195%
26	16.939	2351	2355	2360	rBV2	88275	100833	2.72%	0.209%
27	16.986	2360	2363	2368	rVB2	30191	42660	1.15%	0.088%
28	17.086	2375	2380	2386	rBV7	43398	69136	1.87%	0.143%
29	17.210	2394	2401	2411	rBV2	1935202	2732355	73.75%	5.654%
30	17.310	2411	2418	2424	rVV2	1858778	2601333	70.22%	5.383%
31	17.680	2477	2481	2485	rBV3	62598	79982	2.16%	0.166%
32	17.839	2504	2508	2516	rVB10	45716	82032	2.21%	0.170%
33	17.963	2523	2529	2535	rBV9	45593	89696	2.42%	0.186%
34	18.027	2535	2540	2543	rVV	214017	298684	8.06%	0.618%

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35	18.086	2546	2550	2556	rVV	501577	758349	20.47%	1.569%
36	18.145	2557	2560	2564	rVV5	99632	162232	4.38%	0.336%
37	18.180	2564	2566	2575	rVB8	35600	66908	1.81%	0.138%
38	18.368	2595	2598	2603	rBV3	49300	91515	2.47%	0.189%
39	18.427	2603	2608	2613	rVB4	131795	201863	5.45%	0.418%
40	18.774	2661	2667	2671	rBV8	69508	116971	3.16%	0.242%
41	18.815	2671	2674	2679	rVB7	33979	48697	1.31%	0.101%
42	18.898	2684	2688	2694	rVB8	30055	59517	1.61%	0.123%
43	19.015	2703	2708	2710	rBV5	75197	116106	3.13%	0.240%
44	19.039	2710	2712	2718	rVB4	98461	149865	4.05%	0.310%
45	19.239	2743	2746	2749	rBV3	52979	72725	1.96%	0.150%
46	19.362	2763	2767	2770	rBV2	167974	224068	6.05%	0.464%
47	19.604	2802	2808	2813	rBV	2418574	3297027	89.00%	6.823%
48	19.815	2840	2844	2845	rBV4	37212	49434	1.33%	0.102%
49	19.845	2845	2849	2855	rVB2	345957	536283	14.48%	1.110%
50	19.980	2869	2872	2877	rVB2	153056	199867	5.39%	0.414%
51	20.039	2879	2882	2886	rBV6	42299	63826	1.72%	0.132%
52	20.292	2921	2925	2930	rBV2	233494	330533	8.92%	0.684%
53	20.374	2935	2939	2944	rVV	628492	792702	21.40%	1.640%
54	20.451	2948	2952	2957	rVB3	221200	299324	8.08%	0.619%
55	20.604	2974	2978	2984	rBV8	166483	227569	6.14%	0.471%
56	20.986	3040	3043	3050	rVB5	177347	223034	6.02%	0.462%
57	21.074	3054	3058	3064	rBV	1357408	1576887	42.56%	3.263%
58	21.392	3107	3112	3117	rVB	3049093	3704725	100.00%	7.667%
59	21.974	3207	3211	3218	rVB	1124378	1396639	37.70%	2.890%
60	22.939	3373	3375	3380	rVB	246596	316094	8.53%	0.654%
61	23.550	3472	3479	3489	rVB2	1539040	3226748	87.10%	6.677%
62	23.697	3498	3504	3512	rVB2	1675356	3178527	85.80%	6.578%
63	24.286	3600	3604	3615	rVB4	418701	849806	22.94%	1.759%
64	26.815	4030	4034	4044	rVB8	311852	805102	21.73%	1.666%

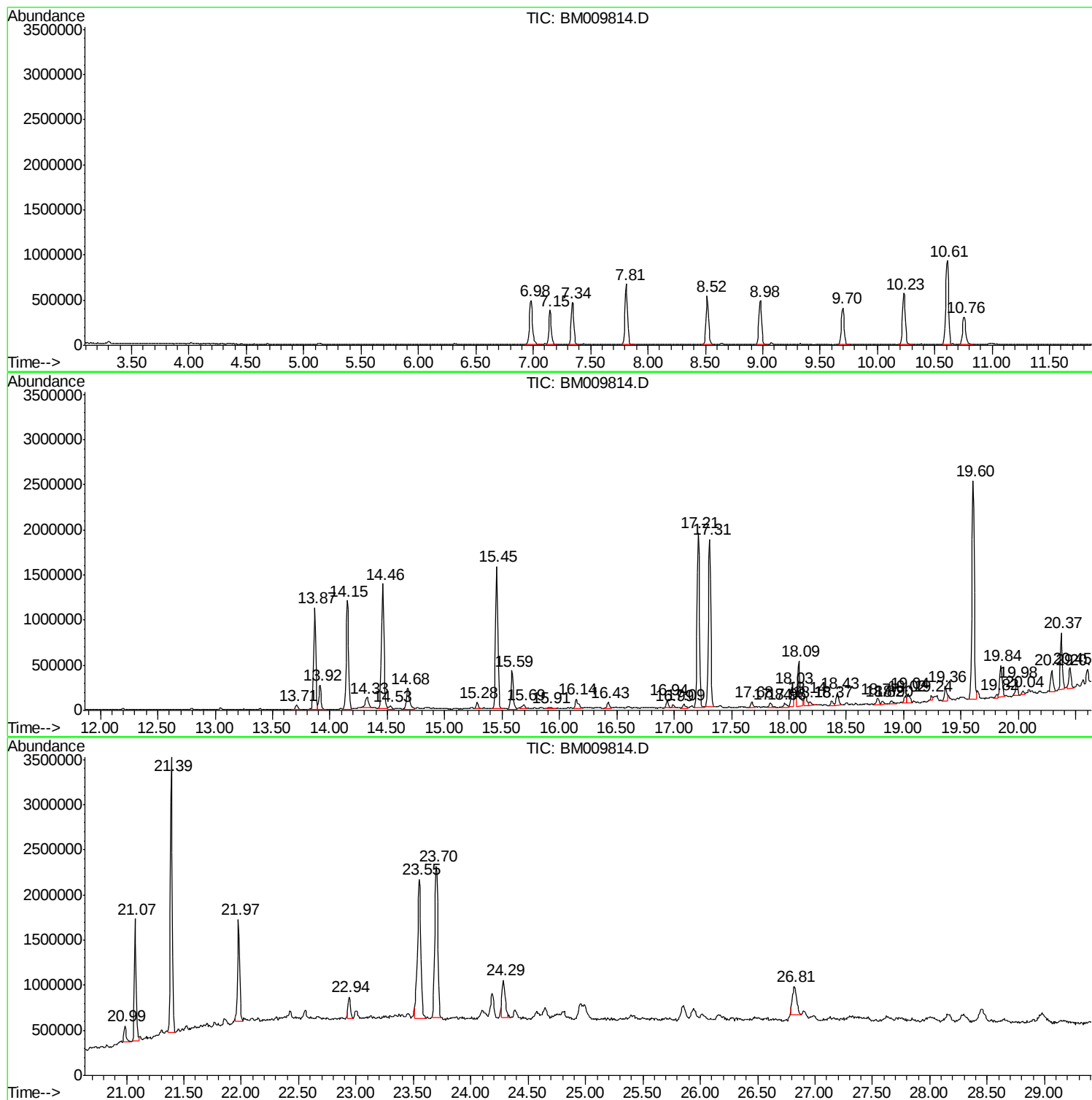
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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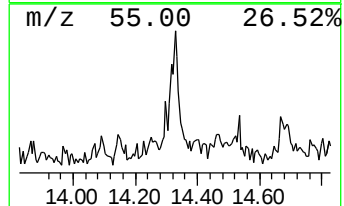
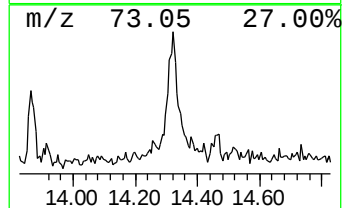
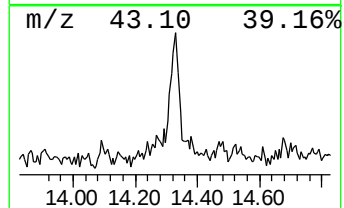
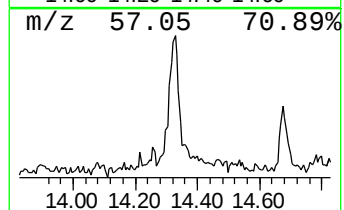
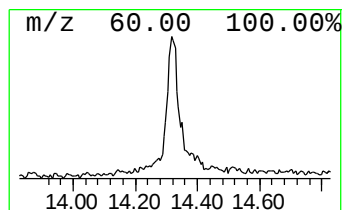
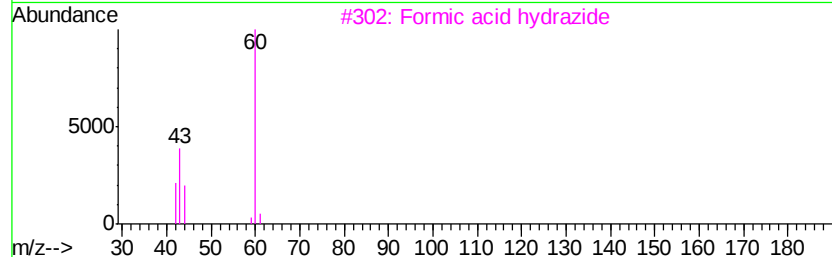
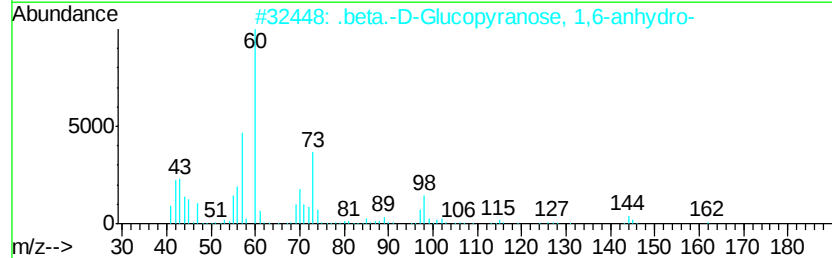
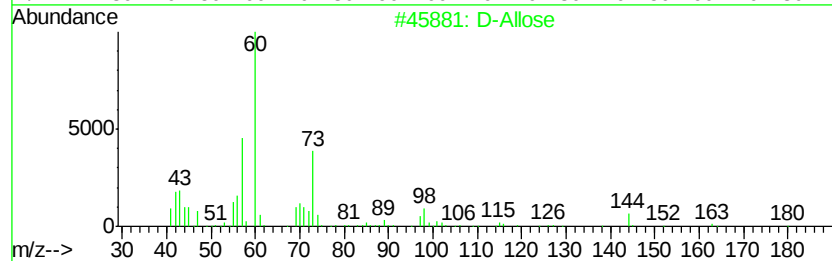
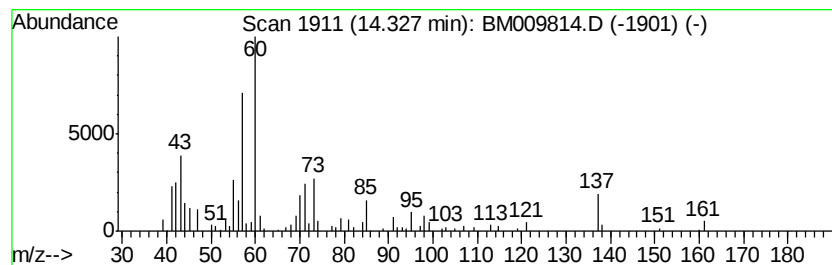
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM042517.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	2.33 ng/ul	257047	Acenaphthene-d10	14.46
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	D-Allose	180 C6H12O6	002595-97-3	43
2	.beta.-D-Glucopyranose, 1,6-anhy...	162 C6H10O5	000498-07-7	40
3	Formic acid hydrazide	60 CH4N2O	000624-84-0	38
4	.beta.-D-Glucopyranose, 1,6-anhy...	162 C6H10O5	000498-07-7	38
5	Silver butanoate	194 C4H7AgO2	005076-24-4	37



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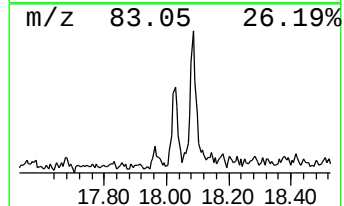
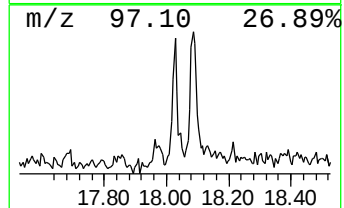
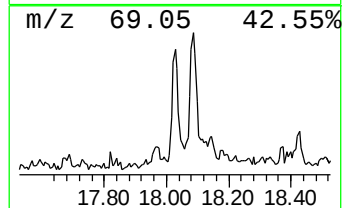
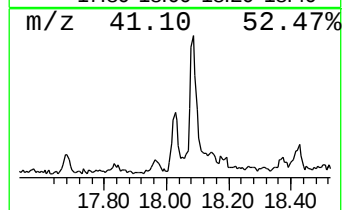
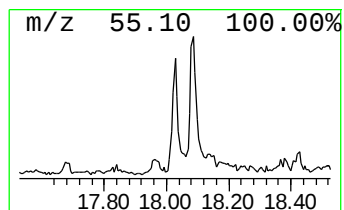
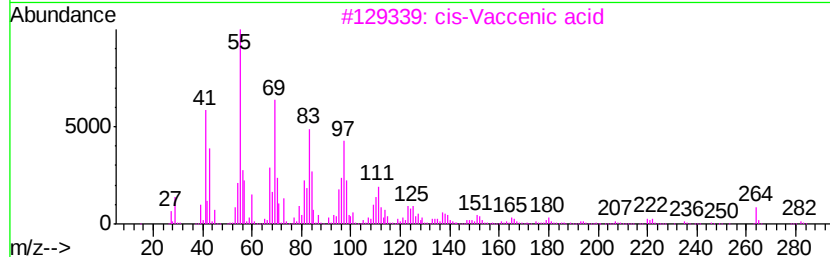
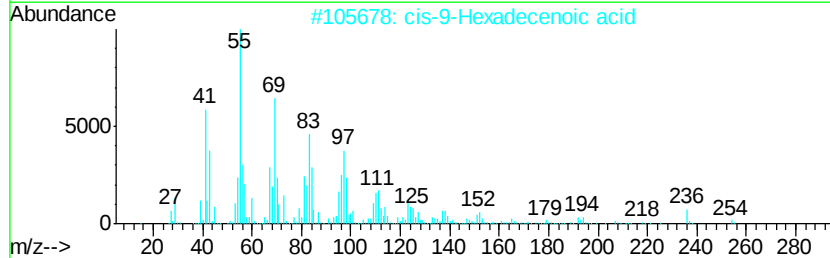
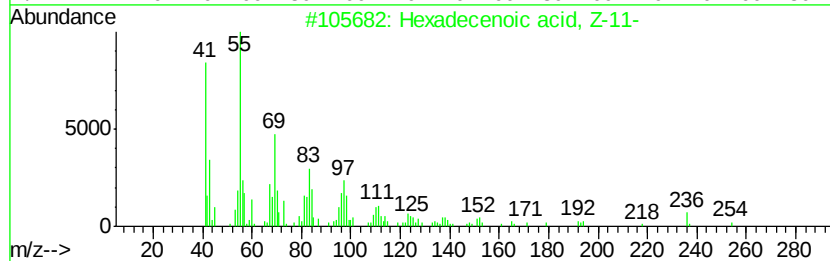
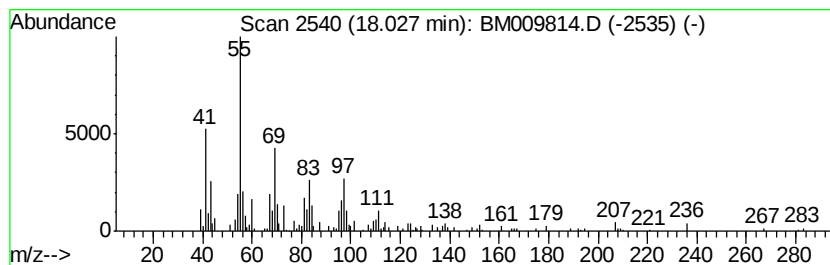
Instrument :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM042517.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Hexadecenoic acid, Z-11- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.		
18.03	2.19 ng/ul	298684	Phenanthrene-d10		17.21		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	87
2			cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	87
3			cis-Vaccenic acid	282	C18H34O2	000506-17-2	86
4			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	78
5			9-Hexadecenoic acid	254	C16H30O2	002091-29-4	72



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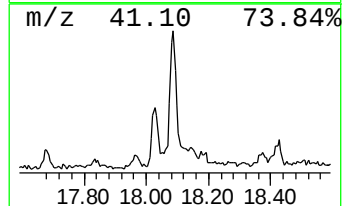
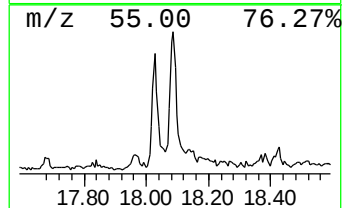
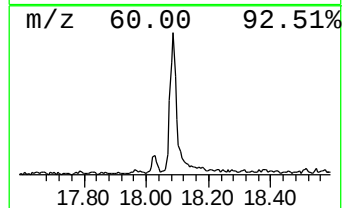
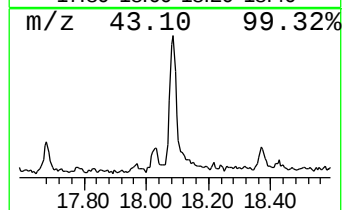
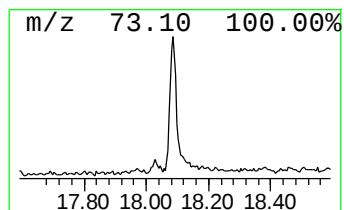
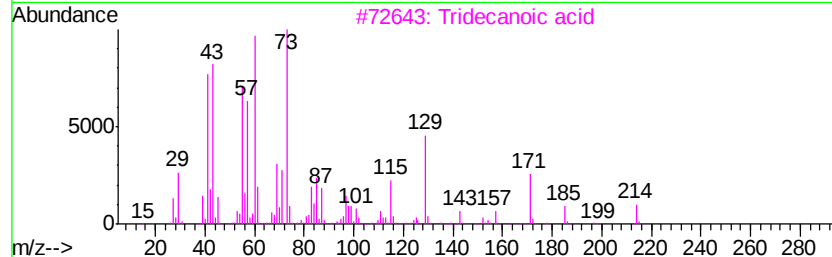
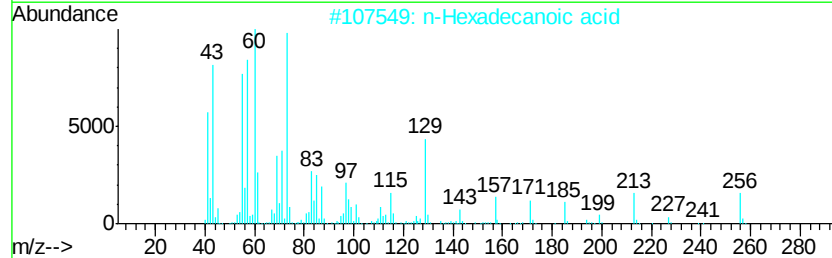
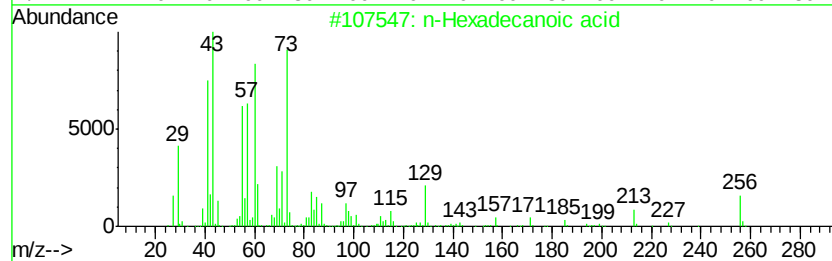
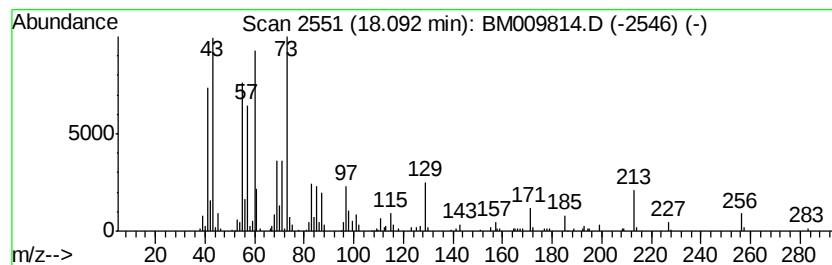
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.09	5.55 ng/ul	758349	Phenanthrene-d10	17.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97	
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95	
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93	
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80	
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74	



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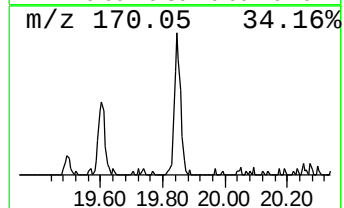
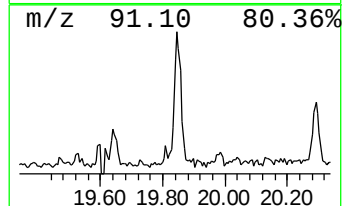
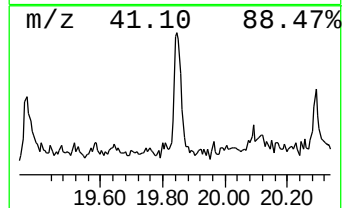
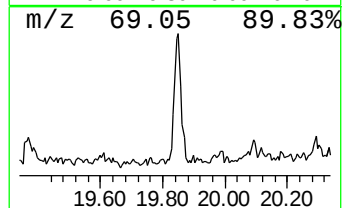
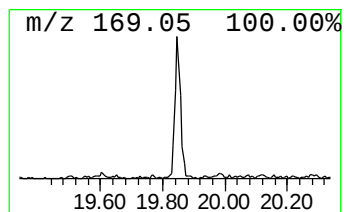
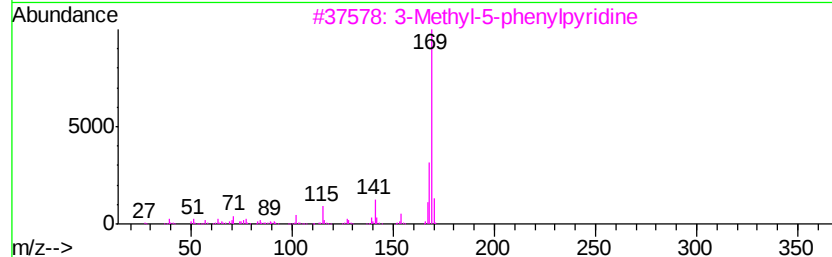
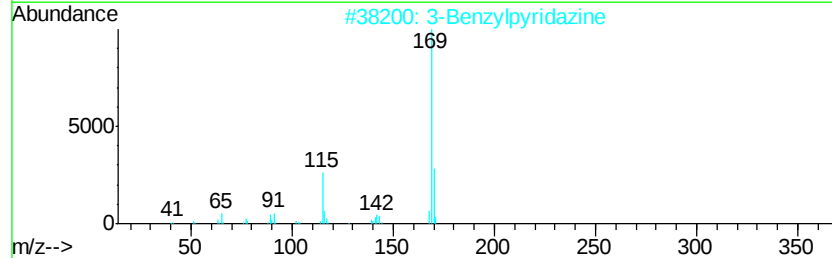
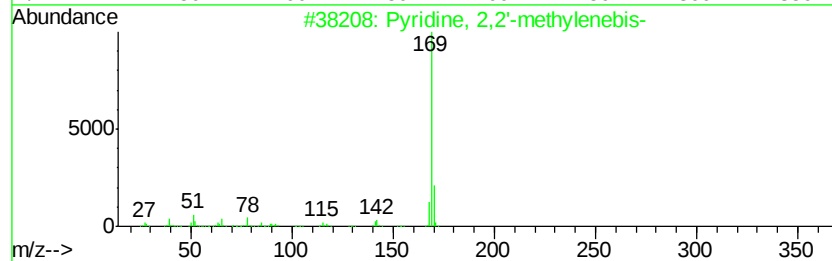
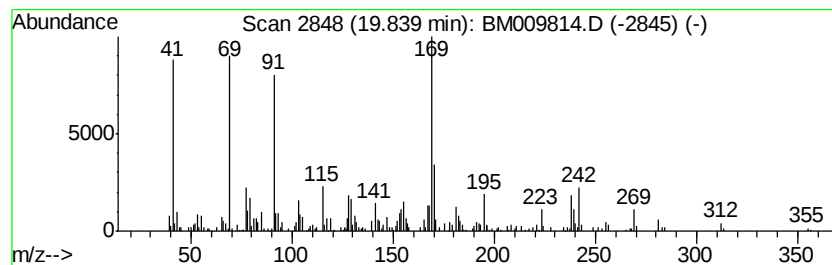
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.84	2.90 ng/ul	536283	Chrysene-d12	21.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyridine, 2,2'-methylenebis-	170	C11H10N2	001132-37-2	43
2		3-Benzylpyridazine	170	C11H10N2	060905-93-3	43
3		3-Methyl-5-phenylpyridine	169	C12H11N	010477-94-8	43
4		[1,1'-Biphenyl]-4-amine	169	C12H11N	000092-67-1	43
5		Pyrimidine-2,4(1H,3H)-dione, 6-h...	169	C6H7N3O3	1000264-12-5	38



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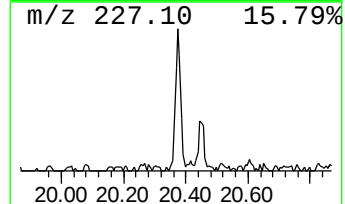
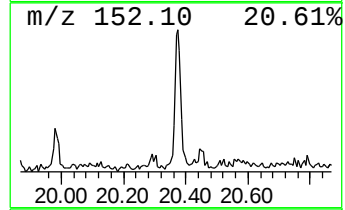
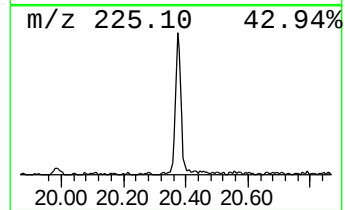
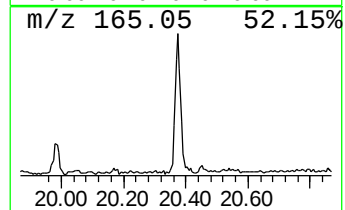
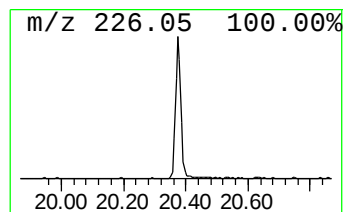
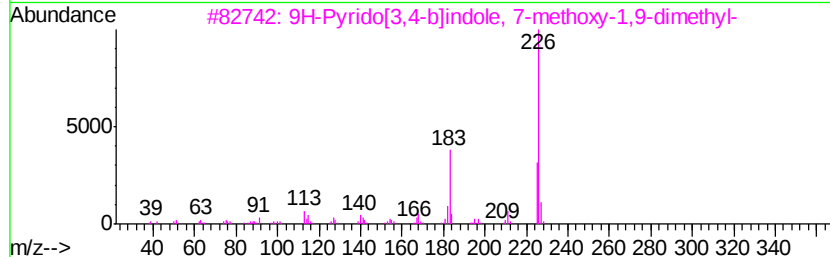
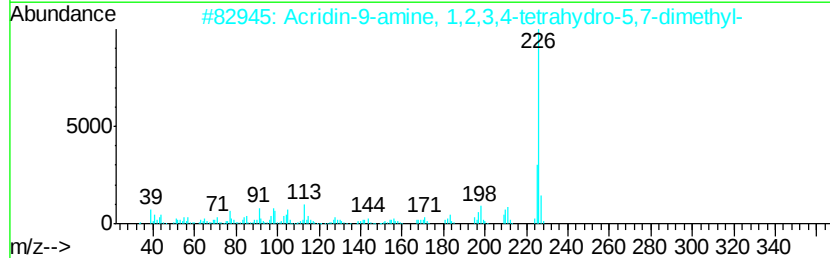
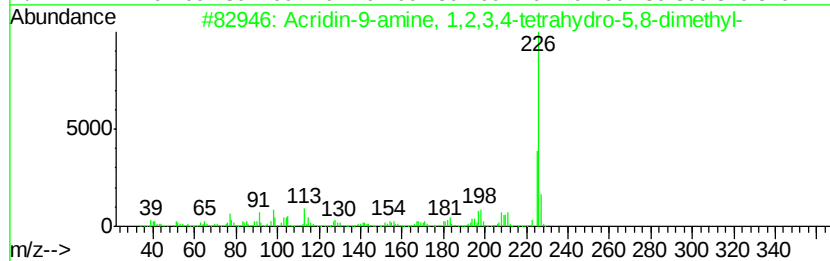
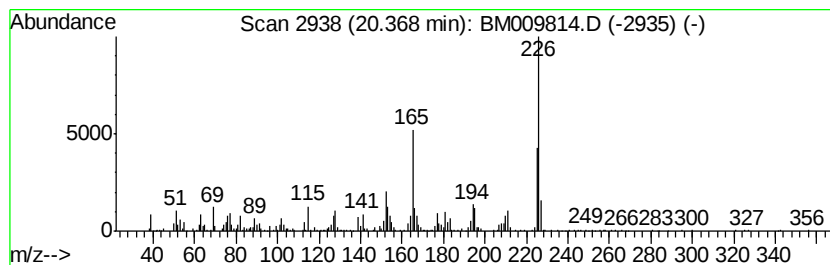
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Acridin-9-amine, 1,2,3,4-te... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.37	4.28 ng/ul	792702	Chrysene-d12	21.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	297758-19-1	58	
2	Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	1000300-57-6	58	
3	9H-Pyrido[3,4-b]indole, 7-methox...	226	C14H14N2O	143502-37-8	52	
4	Benzenamine, N-[(4-nitrophenyl)m...	226	C13H10N2O2	000785-80-8	46	
5	9H-Pyrido[3,4-b]indole, 7-methox...	226	C14H14N2O	143502-37-8	45	



Data Path : Z:\HPCHEM1\BNA M\DATA\BM043017\
Data File : BM009814.D
Acq On : 30 Apr 2017 16:33
Operator : SJ/MA
Sample : I2849-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

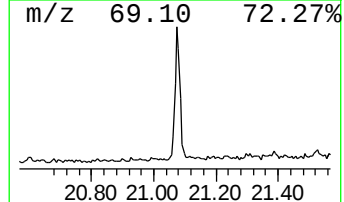
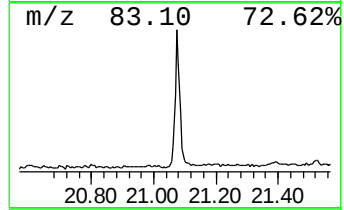
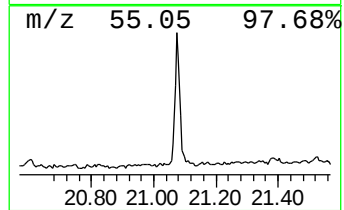
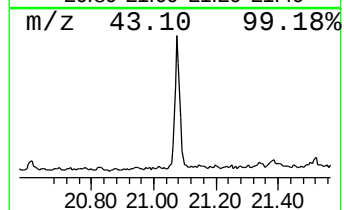
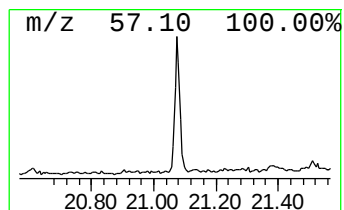
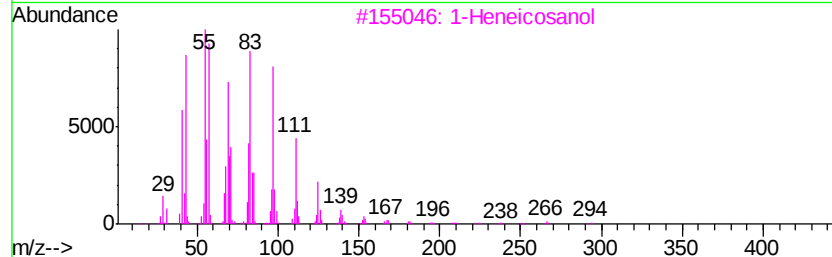
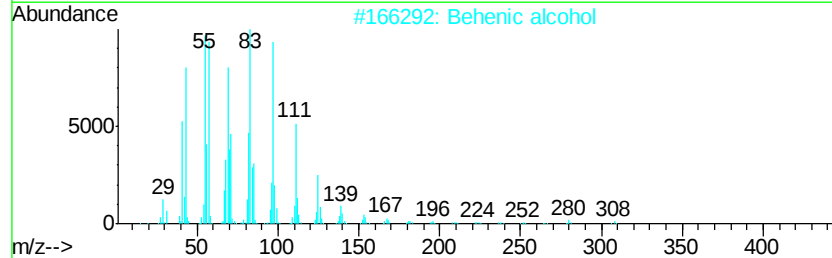
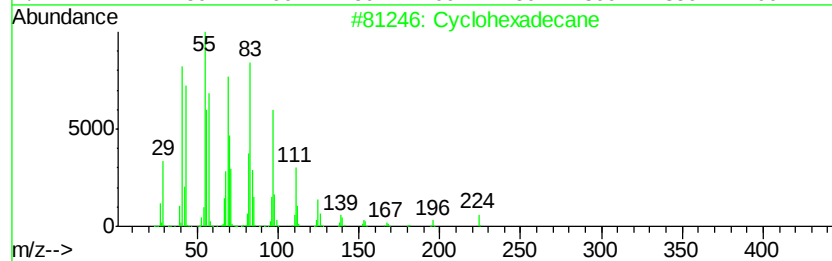
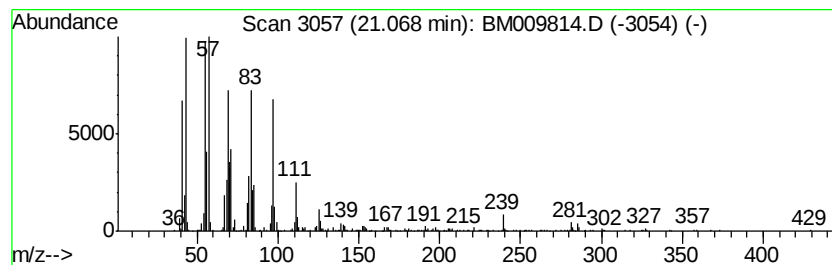
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM042517.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Cyclic21.07 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.	
21.07	8.51 ng/ul	1576890	Chrysene-d12			21.39	
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cvclohexadecane	224	C16H32	000295-65-8	93
2			Behenic alcohol	326	C22H46O	000661-19-8	91
3			1-Heneicosanol	312	C21H44O	015594-90-8	91
4			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\HPCHEM1\BNA M\DATA\BM043017\
Data File : BM009814.D
Acq On : 30 Apr 2017 16:33
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Sample : I2849-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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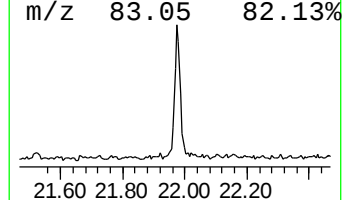
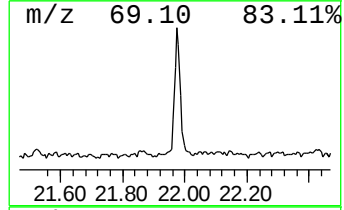
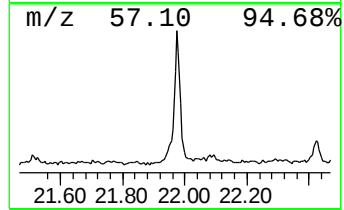
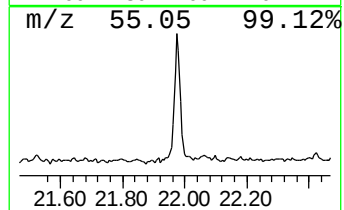
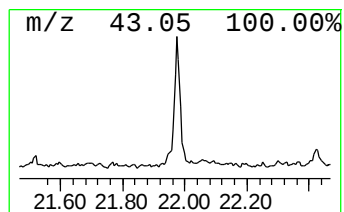
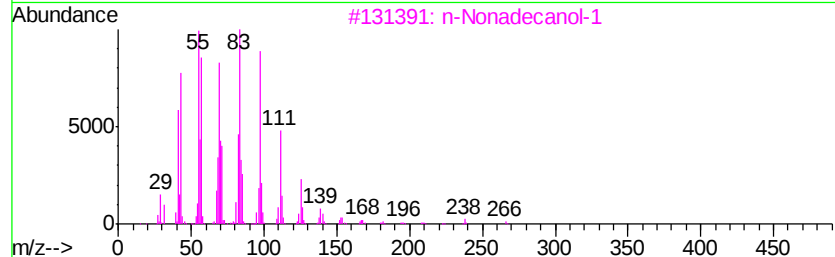
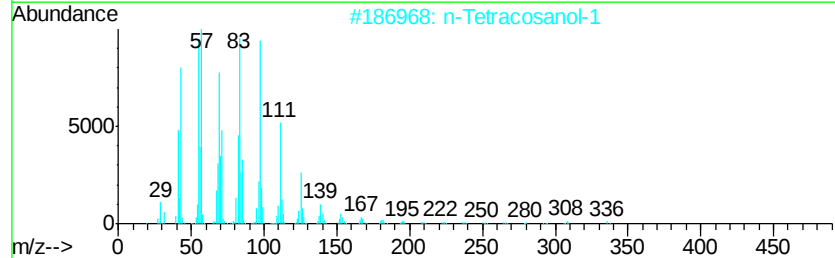
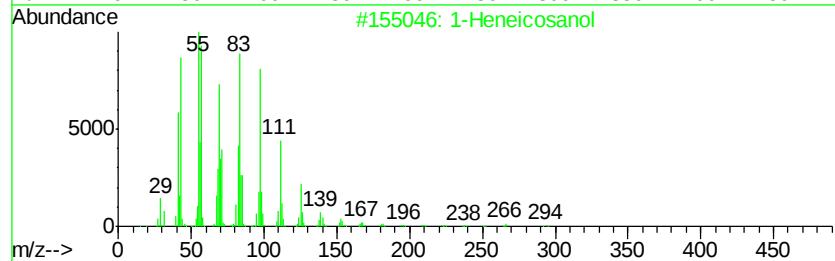
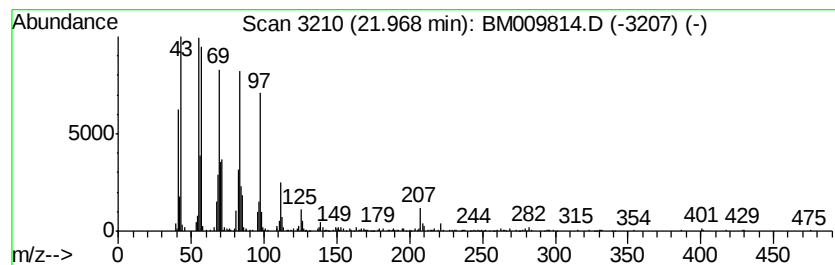
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.97	7.54 ng/ul	1396640	Chrysene-d12	21.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4			1-Heptacosanol	396	C27H56O	002004-39-9	91
5			Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : Z:\HPCHEM1\BNA M\DATA\BM043017\
Data File : BM009814.D
Acq On : 30 Apr 2017 16:33
Operator : SJ/MA
Sample : I2849-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

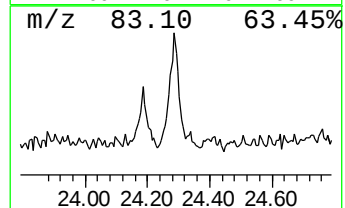
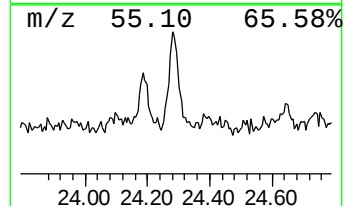
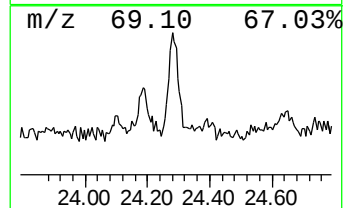
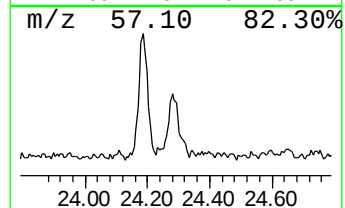
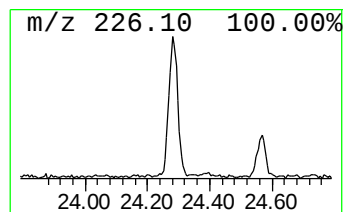
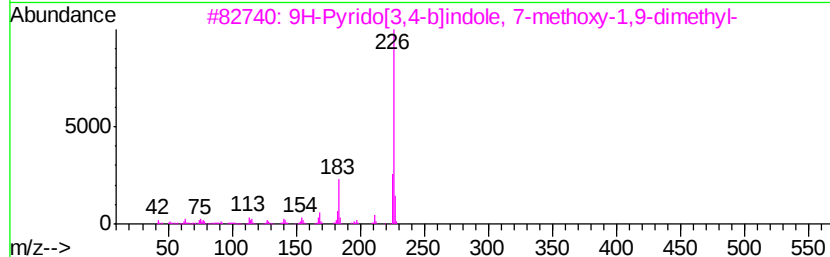
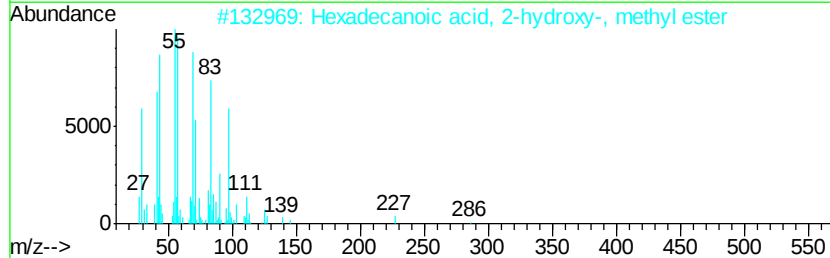
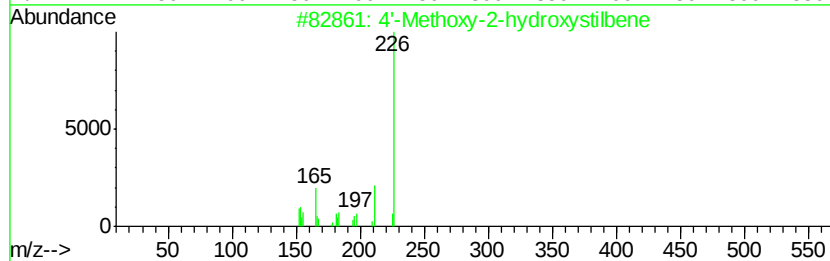
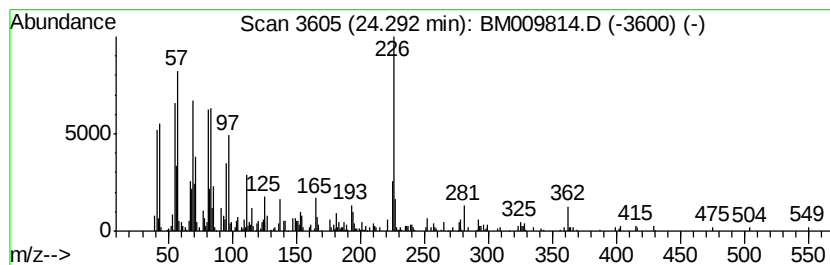
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM042517.M
Quant Title : SVOA CALIBRATION

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

Peak Number 8 4'-Methoxy-2-hydroxystilbene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.29	5.35 ng/ul	849806	Perylene-d12	23.70	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4'-Methoxy-2-hydroxystilbene	226	C15H14O2	1000147-93-1	53
2	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	22
3	9H-Pyrido[3,4-b]indole, 7-methox...	226	C14H14N2O	143502-37-8	20
4	3-Amino-10H-dibenzo[b,f][1,4]oxa...	226	C13H10N2O2	1000311-61-3	18
5	9-Methoxymethyl-1-methyl-3,6-dia...	226	C12H22N2O2	1000216-30-2	18



Data Path : Z:\HPCHEM1\BNA M\DATA\BM043017\
Data File : BM009814.D
Acq On : 30 Apr 2017 16:33
Operator : SJ/MA
Sample : I2849-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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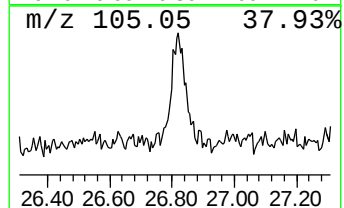
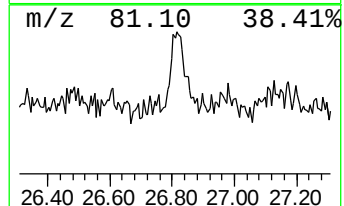
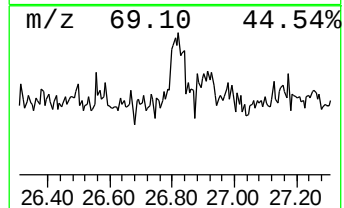
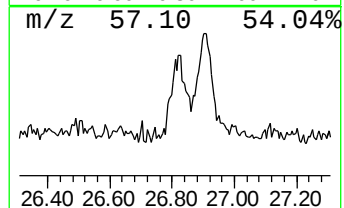
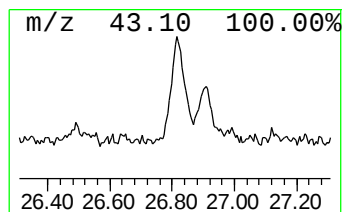
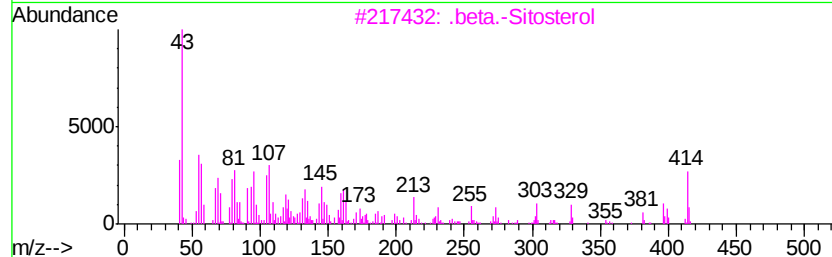
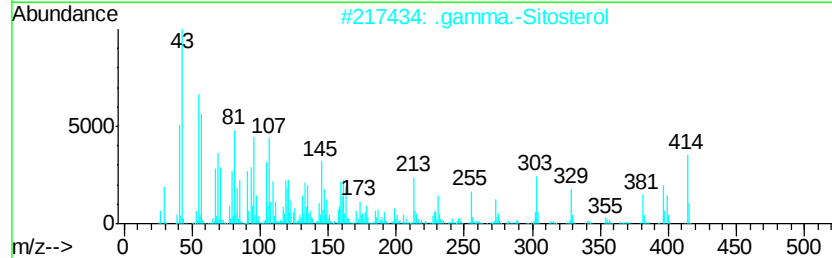
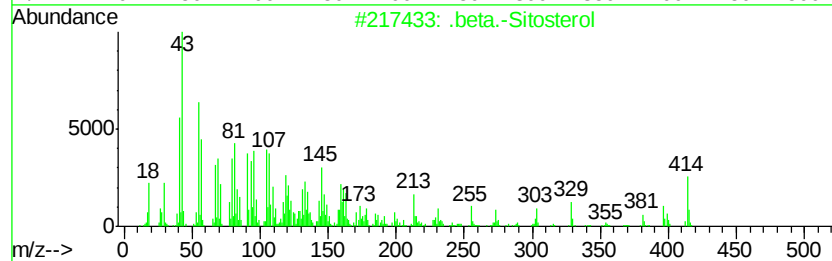
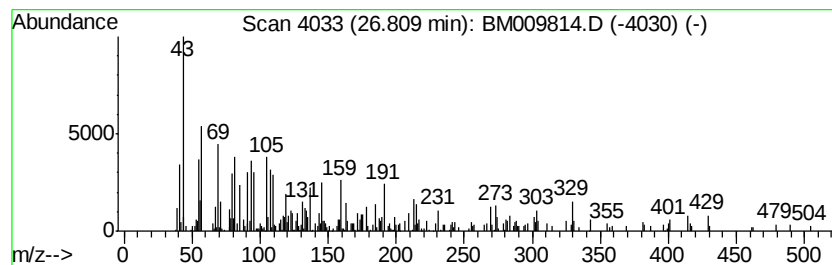
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 unknown-03 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.81	5.07 ng/ul	805102	Perylene-d12	23.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Sitosterol	414	C29H50O	000083-46-5	38
2		.gamma.-Sitosterol	414	C29H50O	000083-47-6	32
3		.beta.-Sitosterol	414	C29H50O	000083-46-5	12
4		Campesterol	400	C28H48O	000474-62-4	11
5		Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	10



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM043017\
Data File : BM009814.D
Acq On : 30 Apr 2017 16:33
Operator : SJ/MA
Sample : I2849-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JHSY3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM042517.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
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Hexadecenoic acid...	18.03	2.2	ng/ul	298684	4	17.21	2732360	20.0
n-Hexadecanoic acid	18.09	5.5	ng/ul	758349	4	17.21	2732360	20.0
unknown-02	19.84	2.9	ng/ul	536283	5	21.39	3704730	20.0
Acridin-9-amine, ...	20.37	4.3	ng/ul	792702	5	21.39	3704730	20.0
(DEL) Alkane: Cyc...	21.07	8.5	ng/ul	1576890	5	21.39	3704730	20.0
1-Heneicosanol	21.97	7.5	ng/ul	1396640	5	21.39	3704730	20.0
4'-Methoxy-2-hydr...	24.29	5.3	ng/ul	849806	6	23.70	3178530	20.0
unknown-03	26.81	5.1	ng/ul	805102	6	23.70	3178530	20.0