

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061219\
 Data File : BM020897.D
 Acq On : 12 Jun 2019 10:34
 Operator : HP/JU
 Sample : K3083-04
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 A51F7

Integration Parameters: LSCINT.P

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

Filtering: 5
 Min Area: 0.1 % 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:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM060619MA.M
 Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.046	5	10	29	rVB	10218137	13396431	100.00%	16.228%
2	3.275	46	49	52	rBV2	24111	33498	0.25%	0.041%
3	3.310	52	55	59	rVB	43108	57314	0.43%	0.069%
4	3.822	139	142	145	rVB	28183	30841	0.23%	0.037%
5	3.934	156	161	166	rVB	80687	114119	0.85%	0.138%
6	4.028	172	177	187	rVB	555786	793033	5.92%	0.961%
7	4.546	262	265	268	rBV4	13989	16743	0.12%	0.020%
8	4.928	326	330	338	rVB	78730	116672	0.87%	0.141%
9	5.034	346	348	356	rVB6	8021	14989	0.11%	0.018%
10	5.457	416	420	425	rBV	27681	46072	0.34%	0.056%
11	5.828	479	483	487	rVB3	17548	26949	0.20%	0.033%
12	5.881	489	492	498	rVB6	7751	14069	0.11%	0.017%
13	6.487	589	595	601	rVB5	17382	32954	0.25%	0.040%
14	6.916	662	668	671	rBV	13268	21035	0.16%	0.025%
15	6.969	671	677	687	rVV	741747	1219411	9.10%	1.477%
16	7.145	701	707	719	rVB	574955	912118	6.81%	1.105%
17	7.339	733	740	750	rBV	790003	1255384	9.37%	1.521%
18	7.804	811	819	827	rBV	926604	1481010	11.06%	1.794%
19	8.051	857	861	868	rVB6	9378	20196	0.15%	0.024%
20	8.504	931	938	950	rBV	886719	1450274	10.83%	1.757%
21	8.633	956	960	965	rVB	13025	18283	0.14%	0.022%
22	8.969	1009	1017	1030	rVV	705520	1156099	8.63%	1.400%
23	9.345	1075	1081	1086	rBV2	13726	21952	0.16%	0.027%
24	9.686	1132	1139	1146	rBV	543461	913789	6.82%	1.107%
25	10.216	1222	1229	1241	rBV	898063	1503777	11.23%	1.822%
26	10.598	1284	1294	1301	rBV	1171442	2005864	14.97%	2.430%
27	10.739	1312	1318	1332	rBV	249644	490274	3.66%	0.594%
28	12.180	1560	1563	1568	rVB3	11959	19590	0.15%	0.024%
29	13.286	1744	1751	1755	rBV5	35224	52253	0.39%	0.063%
30	13.386	1761	1768	1775	rVB8	16347	31515	0.24%	0.038%
31	13.710	1818	1823	1829	rVB6	21357	32379	0.24%	0.039%
32	13.851	1840	1847	1852	rBV	1430673	2064253	15.41%	2.501%
33	13.904	1852	1856	1861	rVB	283147	393421	2.94%	0.477%
34	14.139	1889	1896	1906	rBV	1660273	2491115	18.60%	3.018%

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35	14.274	1912	1919	1925	rVB7	11967	20019	0.15%	0.024%
36	14.445	1936	1948	1955	rBV2	1733004	2604701	19.44%	3.155%
37	14.504	1955	1958	1963	rVB	43947	65023	0.49%	0.079%
38	14.645	1976	1982	1988	rBV	493975	756873	5.65%	0.917%
39	14.804	2005	2009	2013	rBV2	29305	45010	0.34%	0.055%
40	14.845	2013	2016	2024	rVB6	18222	35477	0.26%	0.043%
41	15.286	2088	2091	2098	rVB6	9914	17493	0.13%	0.021%
42	15.439	2110	2117	2123	rBV	2152535	3134299	23.40%	3.797%
43	15.492	2123	2126	2131	rVB3	26704	40643	0.30%	0.049%
44	15.557	2131	2137	2146	rBV	365152	516632	3.86%	0.626%
45	15.674	2151	2157	2164	rVB4	34982	58855	0.44%	0.071%
46	15.786	2171	2176	2179	rBV7	16153	27426	0.20%	0.033%
47	15.898	2191	2195	2198	rBV3	11622	13808	0.10%	0.017%
48	15.927	2198	2200	2206	rVB7	8964	14733	0.11%	0.018%
49	16.157	2234	2239	2242	rBV6	11552	16426	0.12%	0.020%
50	16.345	2266	2271	2275	rVV4	14447	22122	0.17%	0.027%
51	16.586	2307	2312	2316	rBV8	13341	22745	0.17%	0.028%
52	16.845	2352	2356	2361	rBV5	10291	15858	0.12%	0.019%
53	17.009	2380	2384	2388	rVB	23117	30682	0.23%	0.037%
54	17.080	2389	2396	2399	rBV7	12681	25798	0.19%	0.031%
55	17.145	2403	2407	2409	rBV4	11907	15973	0.12%	0.019%
56	17.186	2409	2414	2419	rVV2	2088589	3054613	22.80%	3.700%
57	17.233	2419	2422	2426	rVV	251964	332882	2.48%	0.403%
58	17.286	2426	2431	2443	rVB	2207309	3129208	23.36%	3.791%
59	17.474	2459	2463	2467	rVB6	13859	19586	0.15%	0.024%
60	17.545	2471	2475	2477	rBV	22690	29106	0.22%	0.035%
61	17.592	2481	2483	2487	rVB	23880	30417	0.23%	0.037%
62	17.668	2492	2496	2501	rBV4	35391	54484	0.41%	0.066%
63	17.768	2509	2513	2516	rBV6	12932	20736	0.15%	0.025%
64	17.951	2541	2544	2548	rBV5	13080	21876	0.16%	0.026%
65	18.074	2560	2565	2569	rBV2	282852	404605	3.02%	0.490%
66	18.151	2575	2578	2582	rVB	58544	81882	0.61%	0.099%
67	18.256	2592	2596	2607	rVB3	44989	105815	0.79%	0.128%
68	18.392	2613	2619	2622	rBV	63446	94082	0.70%	0.114%
69	18.562	2646	2648	2652	rVB4	24755	29441	0.22%	0.036%
70	18.609	2653	2656	2660	rVB2	29556	36712	0.27%	0.044%
71	18.945	2711	2713	2716	rBV4	16506	16515	0.12%	0.020%

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72	19.021	2721	2726	2733	rVB2	90448	160874	1.20%	0.195%
73	19.245	2759	2764	2770	rVB	443271	599849	4.48%	0.727%
74	19.356	2779	2783	2788	rBV4	97515	138754	1.04%	0.168%
75	19.580	2815	2821	2835	rBV2	2716787	4392922	32.79%	5.321%
76	20.509	2976	2979	2984	rVB	89289	99668	0.74%	0.121%
77	21.074	3071	3075	3083	rBV	910044	1155837	8.63%	1.400%
78	21.280	3107	3110	3115	rVB	282470	297864	2.22%	0.361%
79	21.368	3119	3125	3129	rBV	2620273	3685990	27.51%	4.465%
80	21.974	3222	3228	3240	rBV2	880745	1544475	11.53%	1.871%
81	22.944	3389	3393	3397	rBV2	567353	927562	6.92%	1.124%
82	22.991	3397	3401	3409	rVB	1176618	2008888	15.00%	2.433%
83	23.509	3483	3489	3501	rVB2	1980706	4068433	30.37%	4.928%
84	23.650	3507	3513	3529	rVB	1922848	3890253	29.04%	4.712%
85	24.185	3600	3604	3611	rVB	450741	806271	6.02%	0.977%
86	24.274	3616	3619	3631	rVB2	401584	864861	6.46%	1.048%
87	26.768	4038	4043	4058	rVB6	593967	1754985	13.10%	2.126%
88	27.556	4169	4177	4187	rBV2	891649	3174213	23.69%	3.845%
89	28.385	4308	4318	4334	rVB2	1569834	5770223	43.07%	6.990%

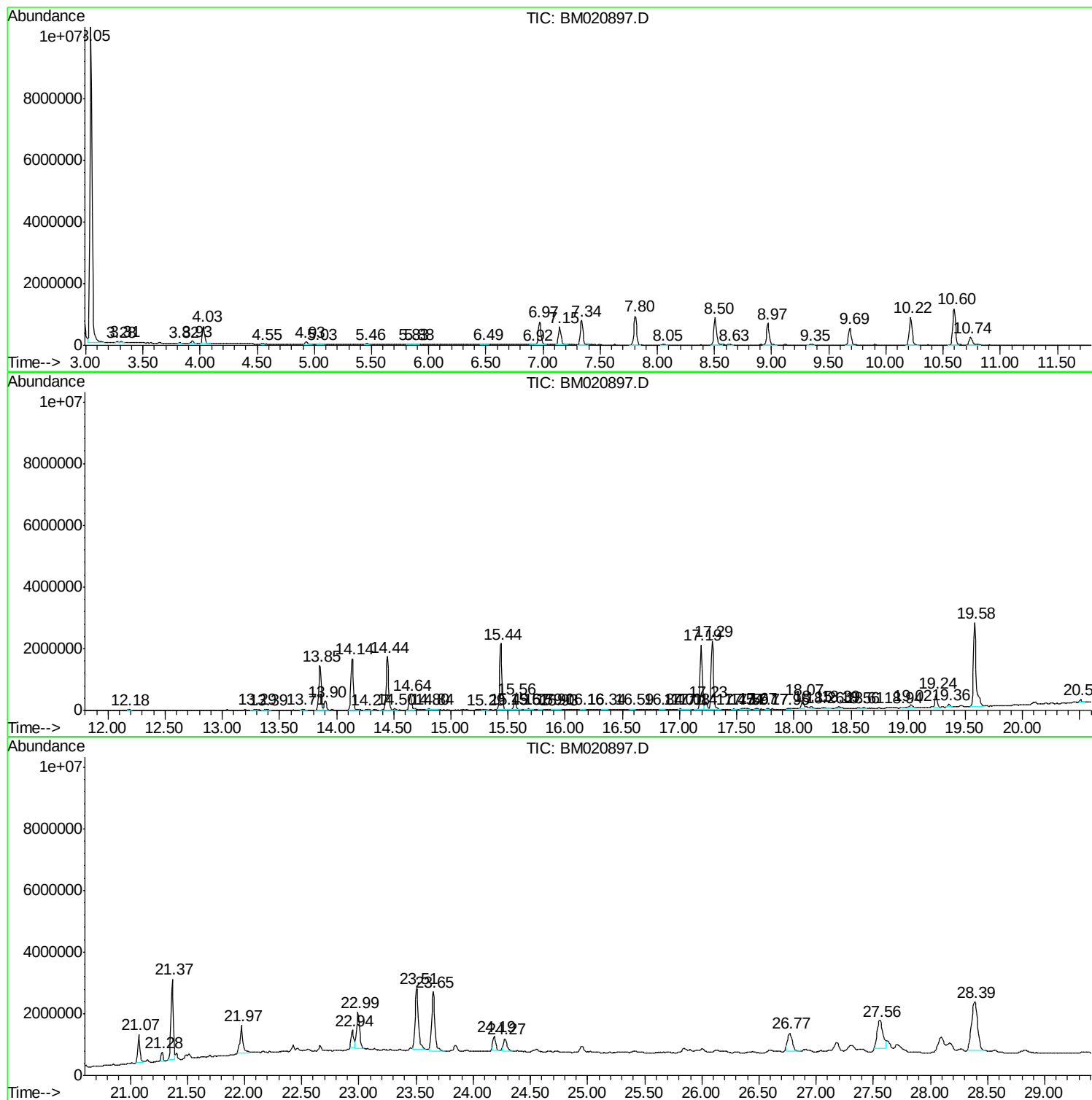
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM060619MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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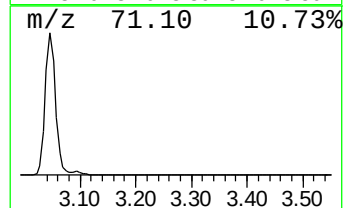
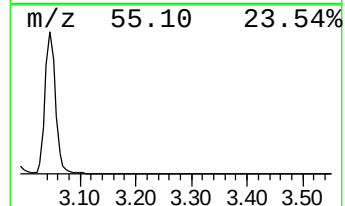
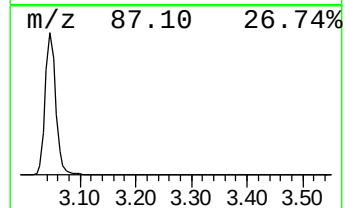
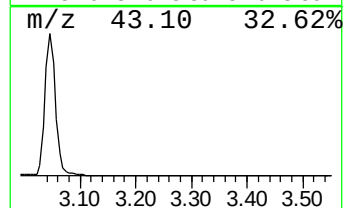
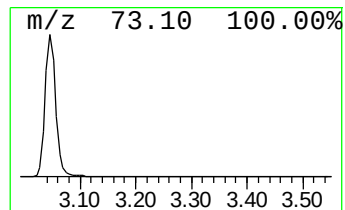
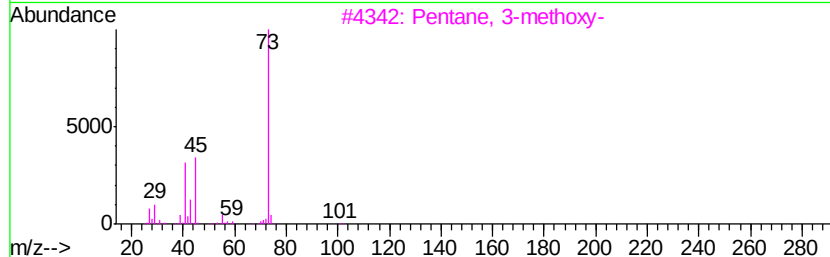
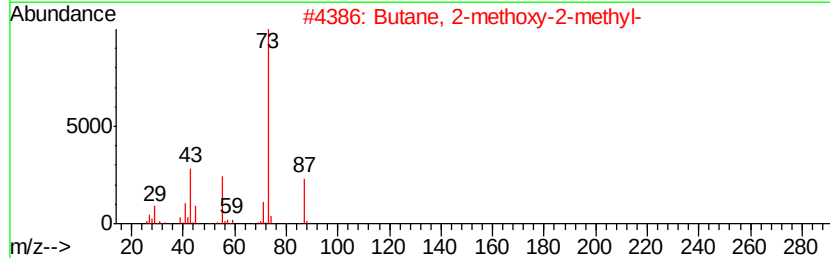
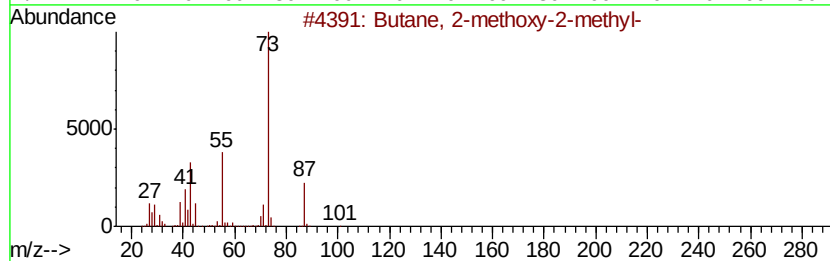
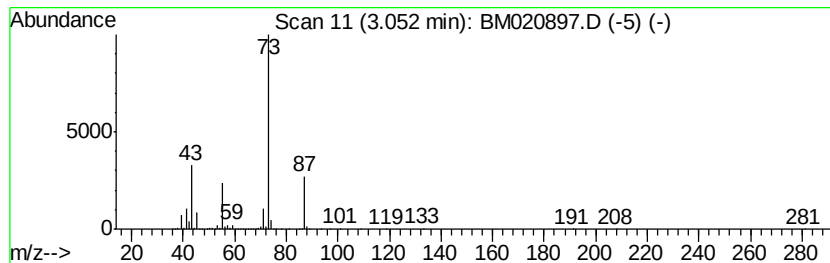
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM060619MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.05	180.91 ng/ul	13396400	1,4-Dichlorobenzene-d4	7.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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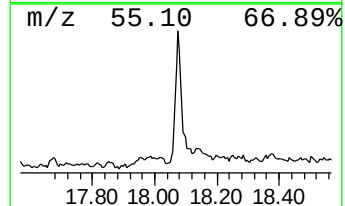
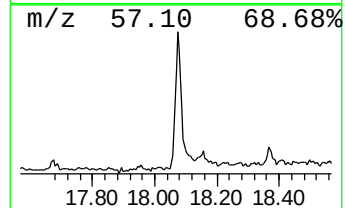
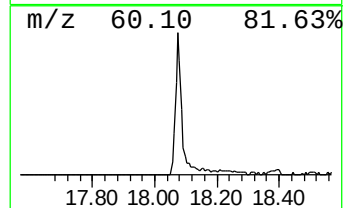
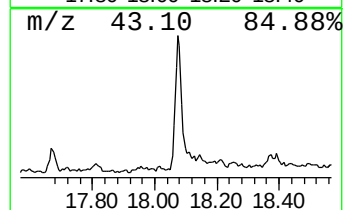
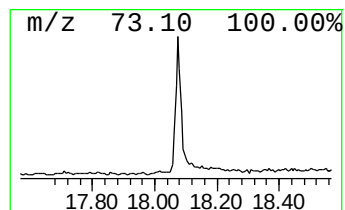
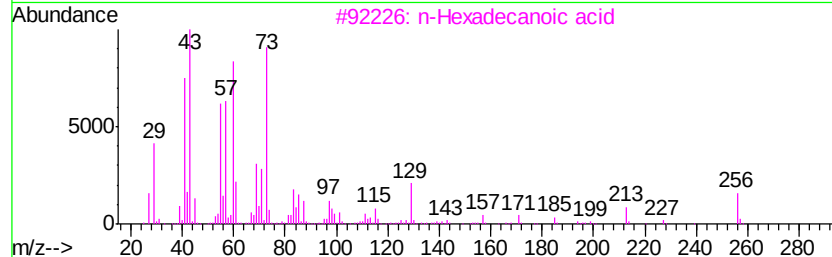
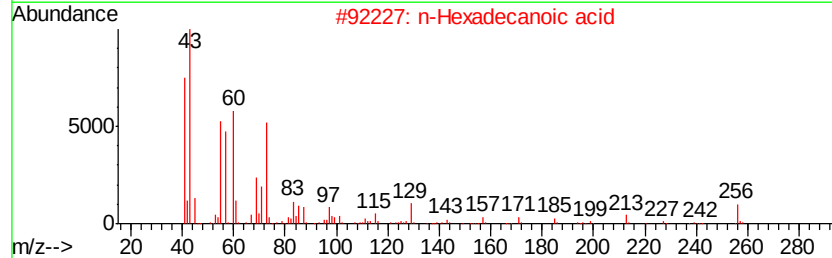
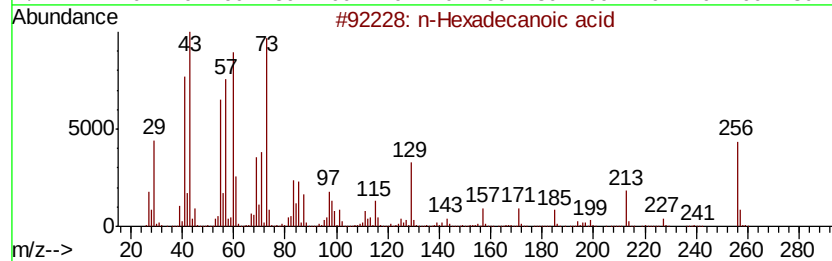
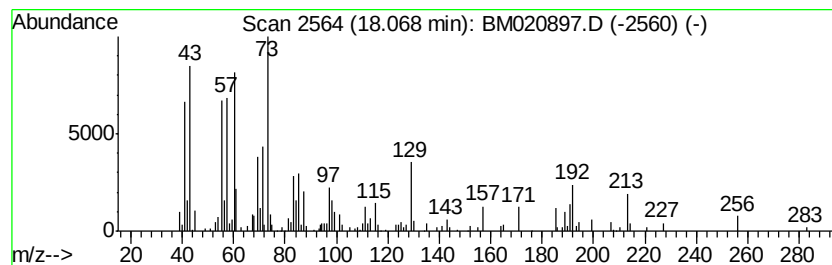
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	2.65 ng/ul	404605	Phenanthrene-d10	17.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4		Tridecanoic acid	214	C13H26O2	000638-53-9	94
5		Tridecanoic acid	214	C13H26O2	000638-53-9	91



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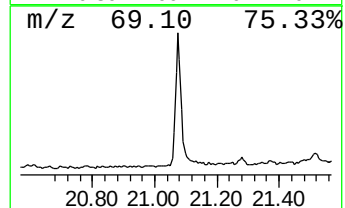
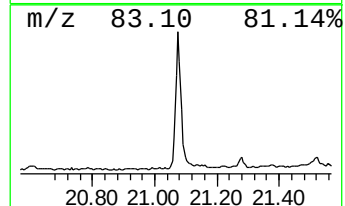
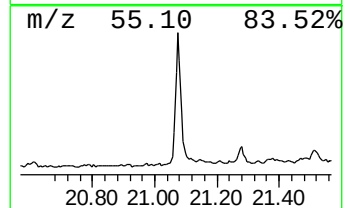
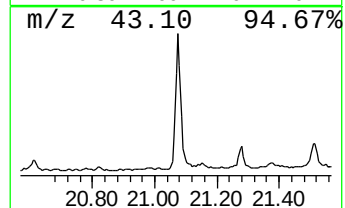
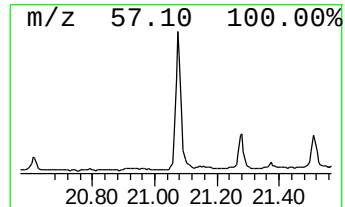
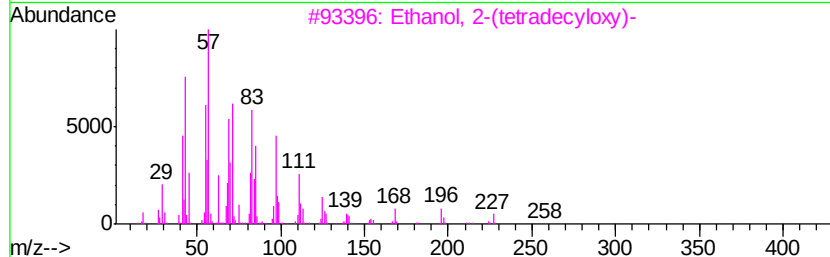
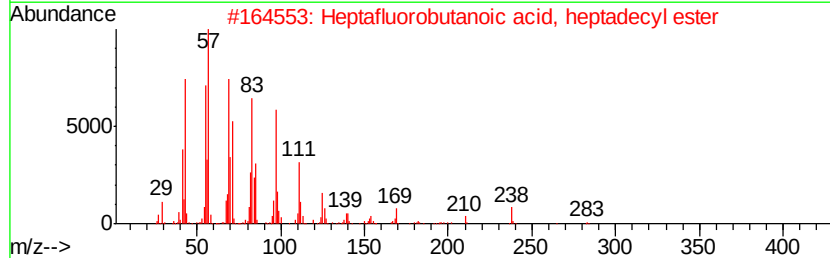
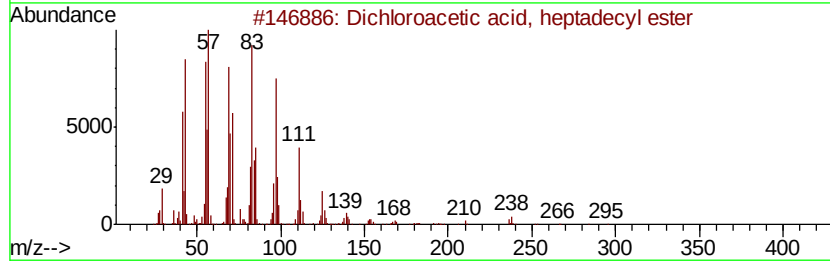
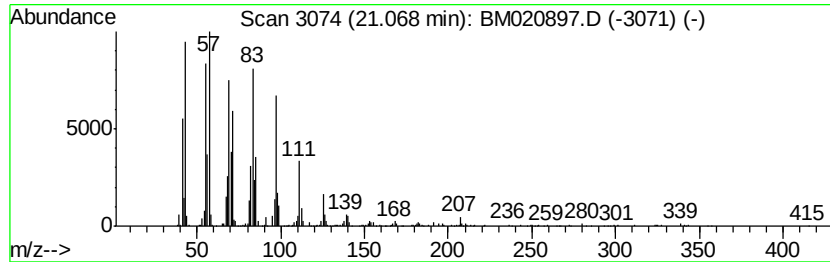
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dichloroacetic acid, heptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.07	6.27 ng/ul	1155840	Chrysene-d12	21.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



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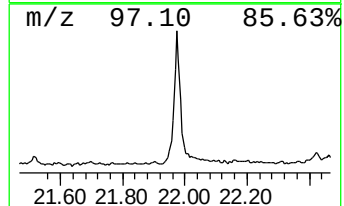
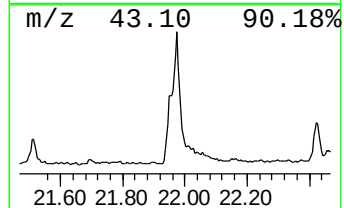
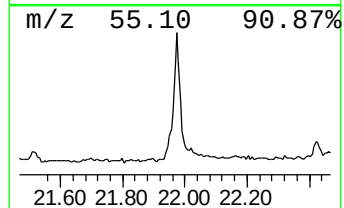
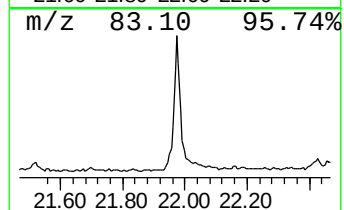
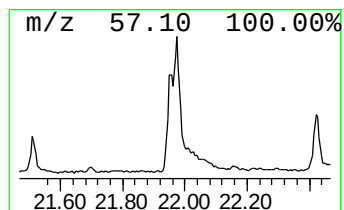
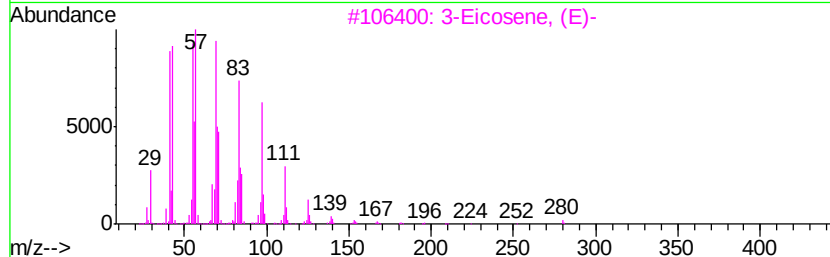
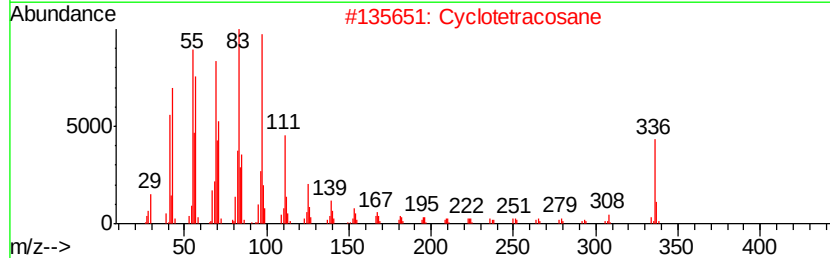
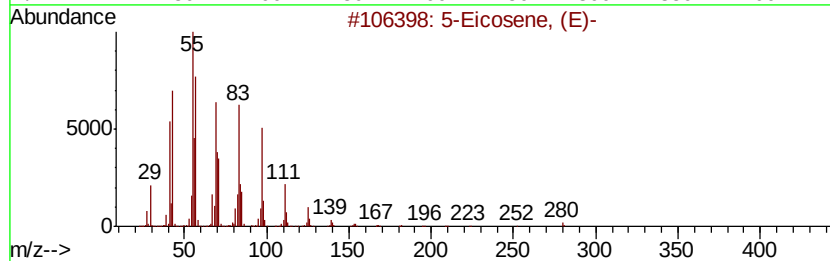
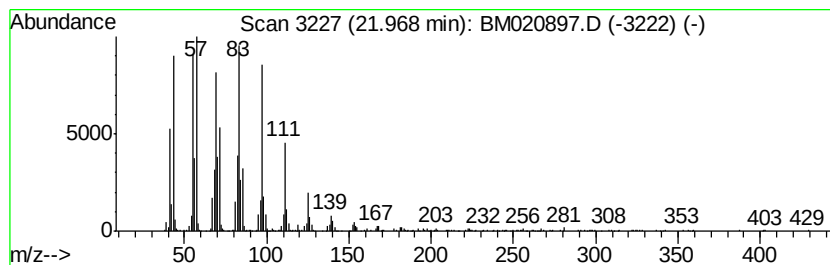
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 (DEL) Alkane: Cyclic21.97 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.97	8.38 ng/ul	1544480	Chrysene-d12	21.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		Cyclotetracosane	336	C24H48	000297-03-0	97
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
5		1-Tricosene	322	C23H46	018835-32-0	89



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061219\
Data File : BM020897.D
Acq On : 12 Jun 2019 10:34
Operator : HP/JU
Sample : K3083-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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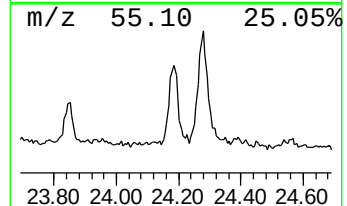
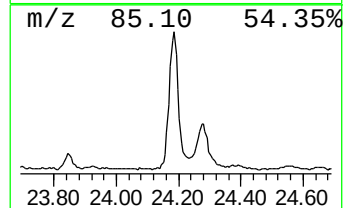
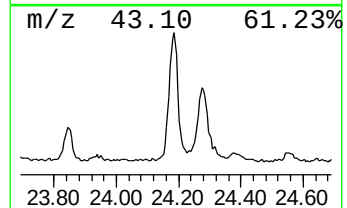
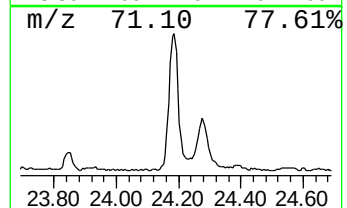
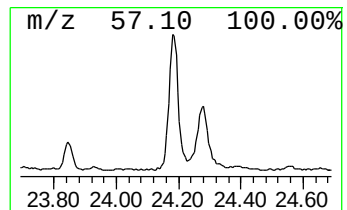
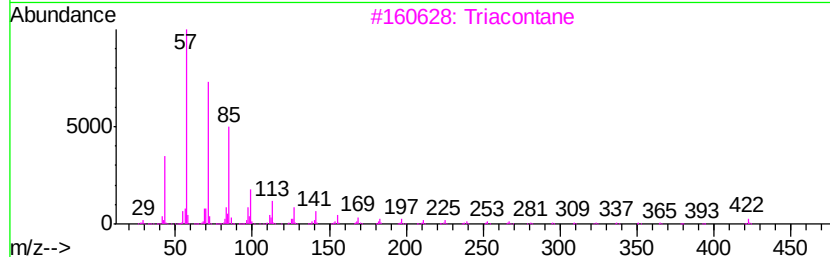
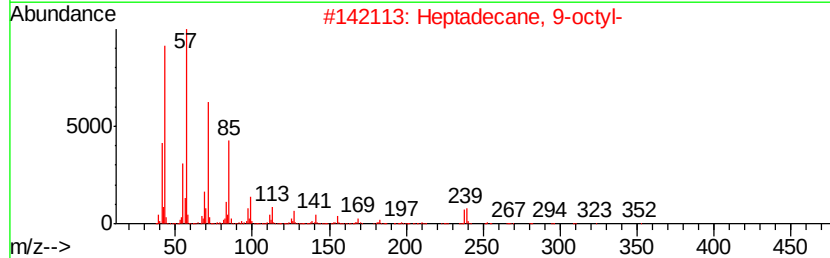
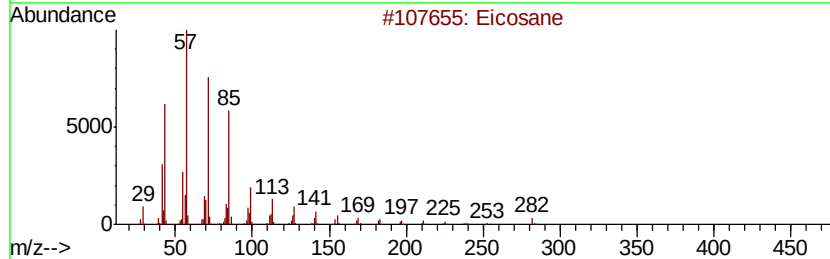
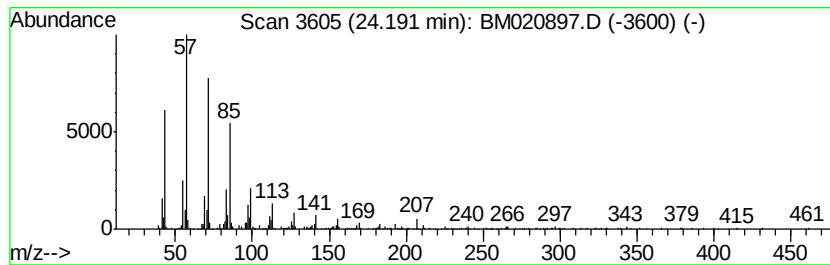
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.19	4.15 ng/ul	806271	Perylene-d12	23.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90
5		Pentacosane	352	C25H52	000629-99-2	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061219\
Data File : BM020897.D
Acq On : 12 Jun 2019 10:34
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Sample : K3083-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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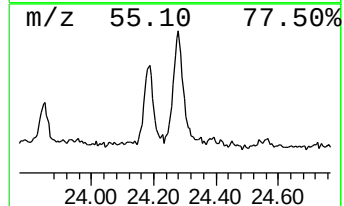
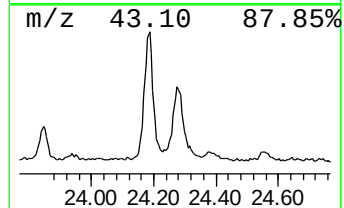
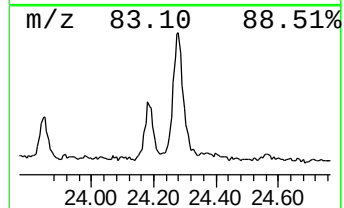
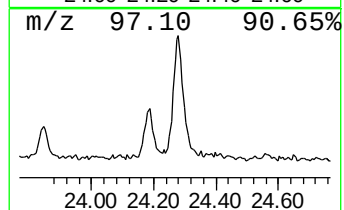
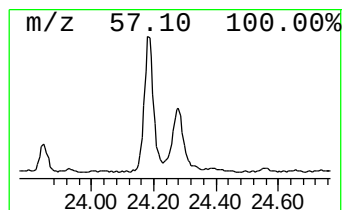
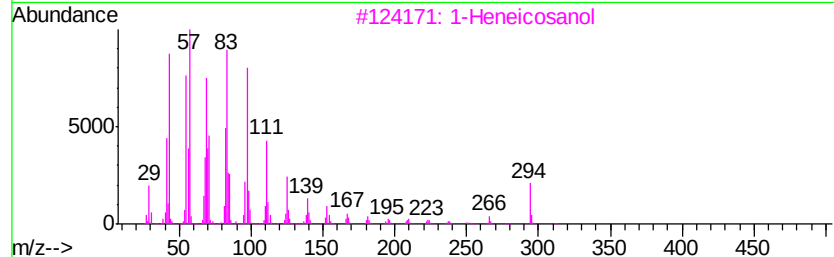
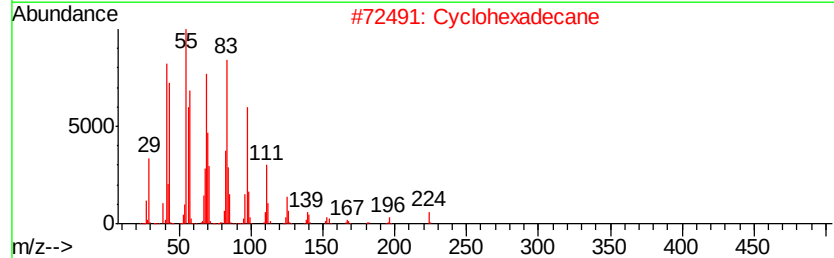
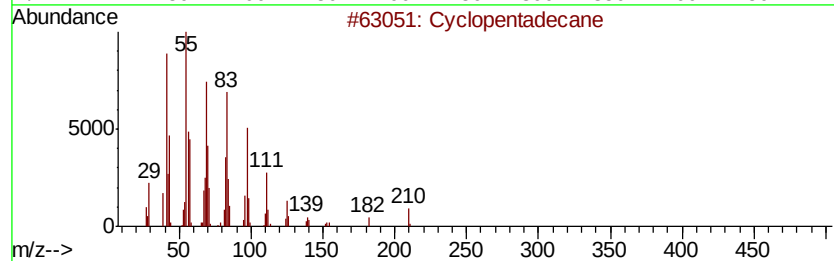
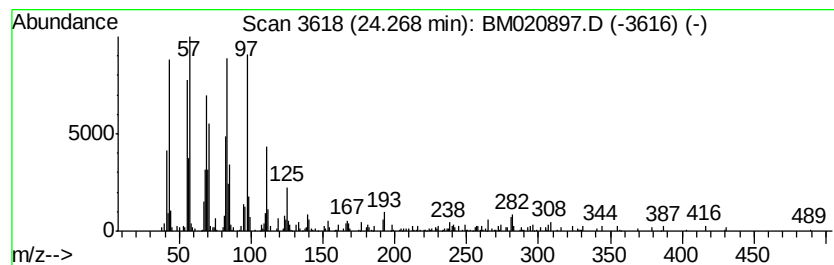
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 (DEL) Alkane: Cyclic24.27 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.27	4.45 ng/ul	864861	Perylene-d12	23.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentadecane	210	C15H30	000295-48-7	96
2		Cyclohexadecane	224	C16H32	000295-65-8	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	94
4		1-Octadecanol	270	C18H38O	000112-92-5	90
5		17-Pentatriacontene	491	C35H70	006971-40-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061219\
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Sample : K3083-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

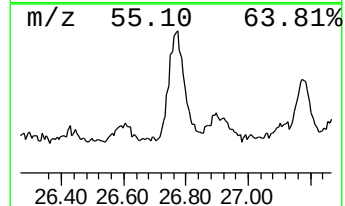
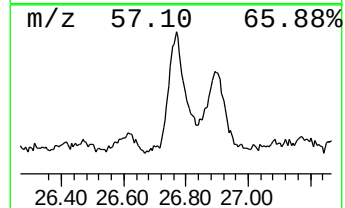
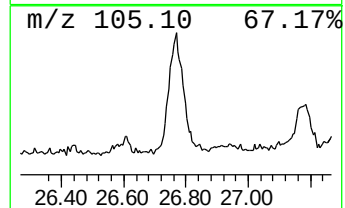
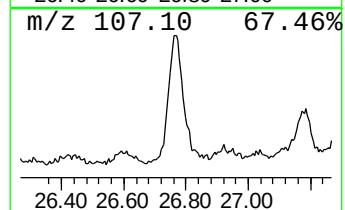
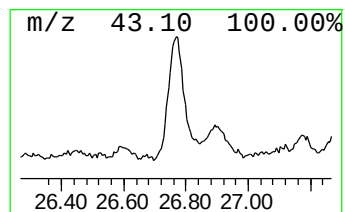
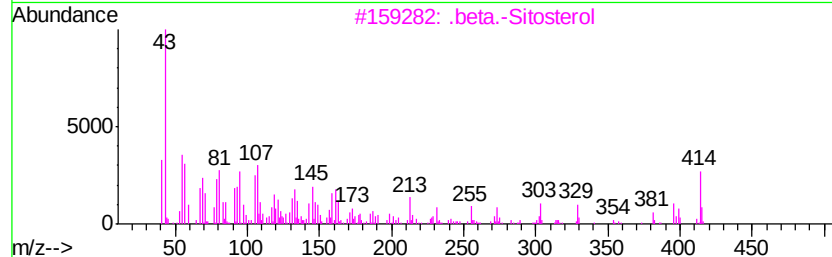
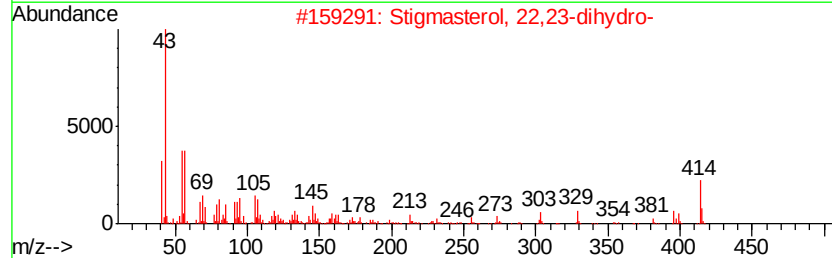
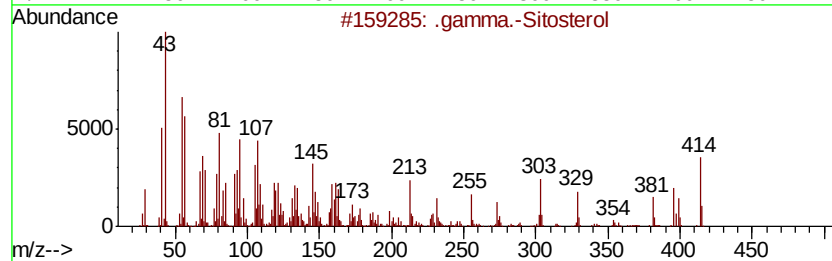
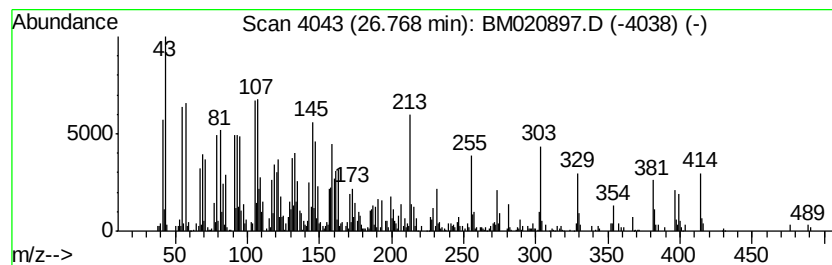
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 .gamma.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.77	9.02 ng/ul	1754990	Perylene-d12	23.65	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	90
2	Stigmasterol, 22,23-dihydro-	414	C29H50O	1000214-20-7	70
3	.beta.-Sitosterol	414	C29H50O	000083-46-5	46
4	.beta.-Sitosterol	414	C29H50O	000083-46-5	38
5	.beta.-Sitosterol	414	C29H50O	000083-46-5	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061219\
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Sample : K3083-04
Misc :
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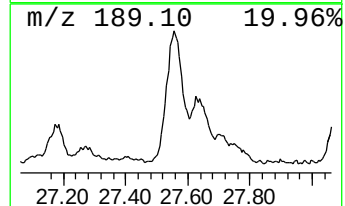
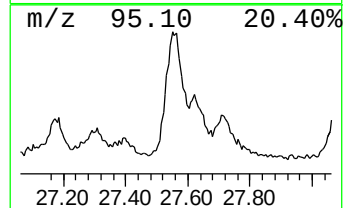
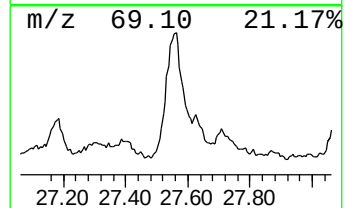
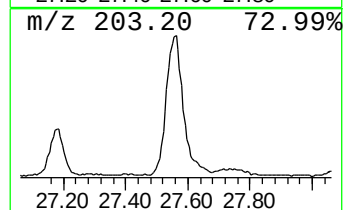
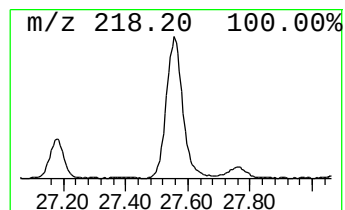
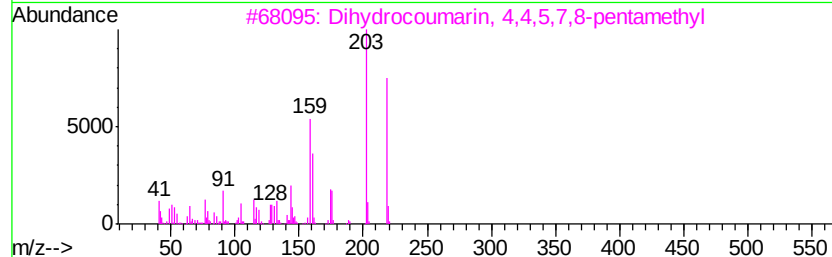
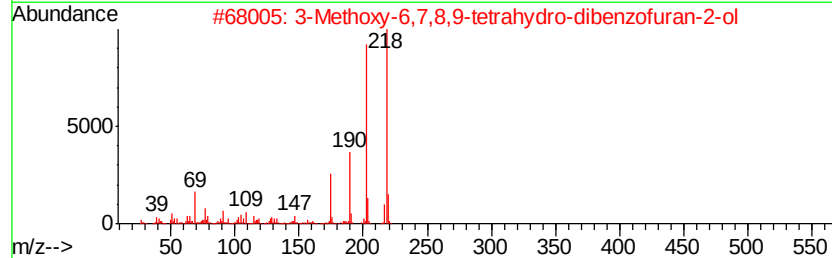
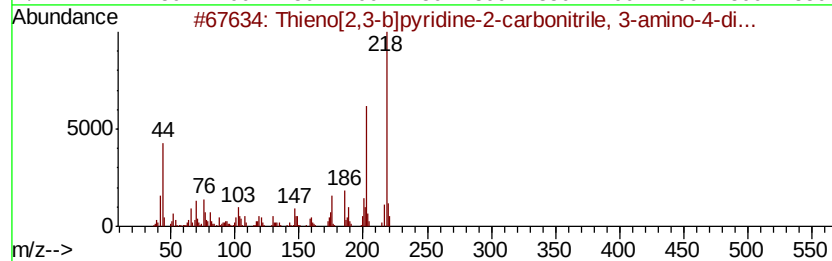
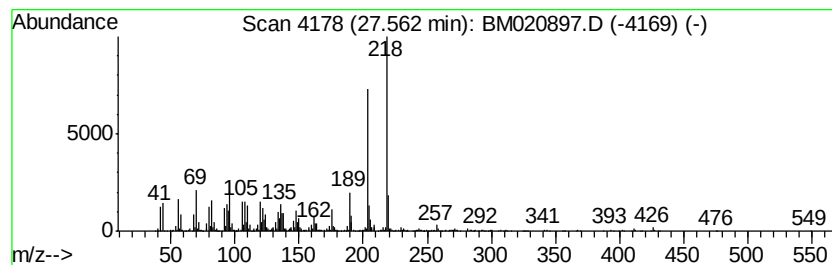
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Thieno[2,3-b]pyridine-2-car... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
27.56	16.32 ng/ul	3174210	Perylene-d12	23.65		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thieno[2,3-b]pyridine-2-carbonit...	218	C10H10N4S	147992-88-9	72	
2	3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	68	
3	Dihydrocoumarin, 4,4,5,7,8-penta...	218	C14H18O2	039170-97-3	59	
4	5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	53	
5	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	52	



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061219\
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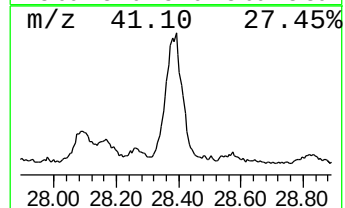
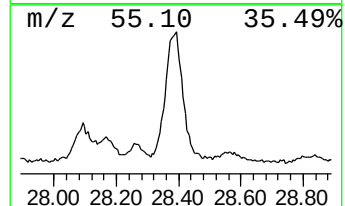
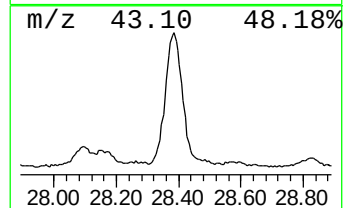
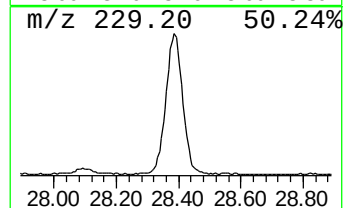
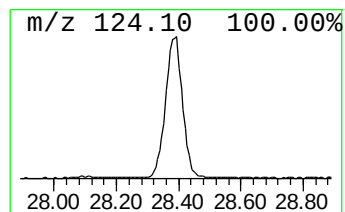
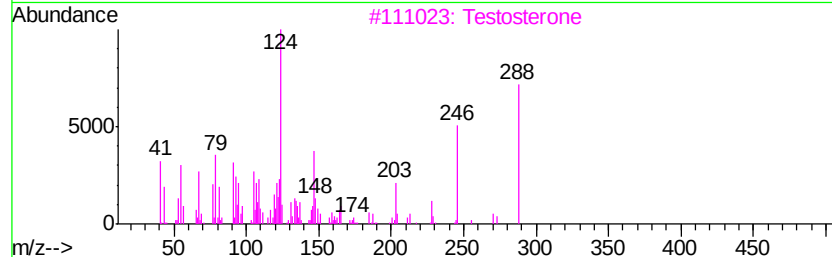
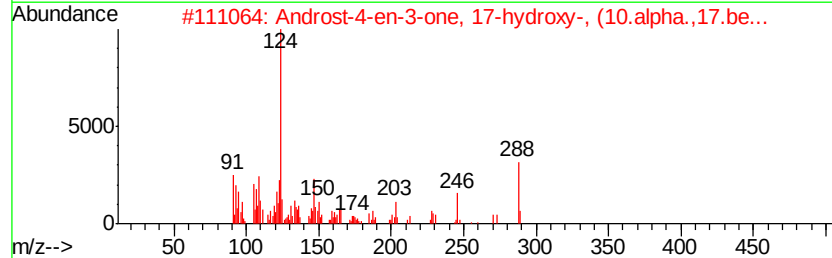
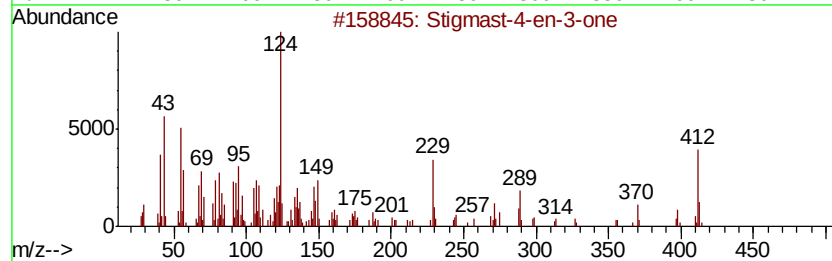
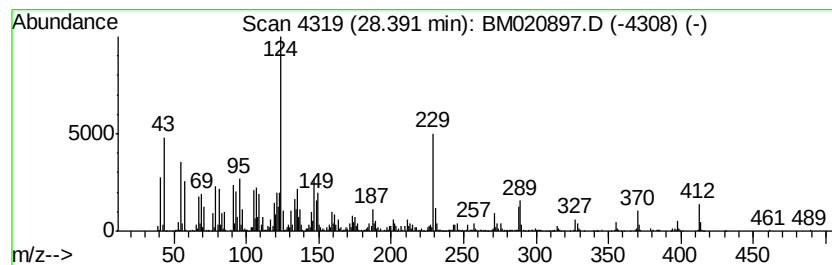
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Stigmast-4-en-3-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.39	29.67 ng/ul	5770220	Perylene-d12	23.65
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Stigmast-4-en-3-one	412 C29H48O	001058-61-3 94
2		Androst-4-en-3-one, 17-hydroxy-, ...	288 C19H28O2	000604-39-7 64
3		Testosterone	288 C19H28O2	000058-22-0 64
4		Testosterone	288 C19H28O2	000058-22-0 64
5		Testosterone	288 C19H28O2	000058-22-0 45



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM061219\
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Sample : K3083-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

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ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.05	180.9	ng/ul	13396400	1	7.80	1481010	20.0
n-Hexadecanoic acid	18.07	2.6	ng/ul	404605	4	17.19	3054610	20.0
Dichloroacetic ac...	21.07	6.3	ng/ul	1155840	5	21.37	3685990	20.0
(DEL) Alkane: Cyc...	21.97	8.4	ng/ul	1544480	5	21.37	3685990	20.0
(DEL) Alkane: Str...	24.19	4.2	ng/ul	806271	6	23.65	3890250	20.0
(DEL) Alkane: Cyc...	24.27	4.5	ng/ul	864861	6	23.65	3890250	20.0
.gamma.-Sitosterol	26.77	9.0	ng/ul	1754990	6	23.65	3890250	20.0
Thieno[2,3-b]pyri...	27.56	16.3	ng/ul	3174210	6	23.65	3890250	20.0
Stigmast-4-en-3-one	28.39	29.7	ng/ul	5770220	6	23.65	3890250	20.0