

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082517\
 Data File : BG082506.D
 Acq On : 26 Aug 2017 00:59
 Operator : SJ/JU
 Sample : I4885-07
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B0AQ7

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.1
 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: 1

Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.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	3.734	18	25	35	rVV	134192	229706	13.91%	1.270%
2	3.816	35	39	47	rVB5	10887	21432	1.30%	0.118%
3	3.893	50	52	55	rVB3	2617	2961	0.18%	0.016%
4	3.922	55	57	62	rBV3	2839	3185	0.19%	0.018%
5	4.075	76	83	89	rBV8	5951	13199	0.80%	0.073%
6	4.551	160	164	167	rBV6	2492	2976	0.18%	0.016%
7	4.668	183	184	188	rBV4	2712	3195	0.19%	0.018%
8	4.733	192	195	201	rVB4	2771	5103	0.31%	0.028%
9	4.862	209	217	227	rBV6	10925	23152	1.40%	0.128%
10	4.938	227	230	234	rVB4	3258	4037	0.24%	0.022%
11	5.050	246	249	254	rBV4	2156	4043	0.24%	0.022%
12	5.444	307	316	325	rBV	54411	88125	5.34%	0.487%
13	6.401	474	479	486	rVB5	3993	8012	0.49%	0.044%
14	6.554	497	505	511	rVB5	1749	3266	0.20%	0.018%
15	7.324	631	636	644	rBV5	4477	8875	0.54%	0.049%
16	7.494	656	665	678	rBV	229756	468599	28.37%	2.590%
17	7.653	684	692	700	rBV	167036	283290	17.15%	1.566%
18	7.870	720	729	748	rVB	225072	407977	24.70%	2.255%
19	8.340	800	809	820	rBV	142174	245166	14.84%	1.355%
20	8.652	858	862	869	rVV5	2661	6416	0.39%	0.035%
21	9.034	916	927	940	rBV2	289000	531061	32.15%	2.935%
22	9.351	978	981	987	rBV2	1792	4105	0.25%	0.023%
23	9.504	996	1007	1018	rBV	227595	435837	26.39%	2.409%
24	9.604	1018	1024	1028	rBV6	4565	9003	0.55%	0.050%
25	10.232	1121	1131	1141	rBV	197163	378554	22.92%	2.092%
26	10.450	1161	1168	1174	rBV6	7814	19412	1.18%	0.107%
27	10.667	1200	1205	1208	rVB2	2824	4156	0.25%	0.023%
28	10.779	1216	1224	1241	rBV	290452	583452	35.32%	3.225%
29	11.025	1258	1266	1268	rVB3	1784	3578	0.22%	0.020%
30	11.161	1281	1289	1302	rVV	201966	374470	22.67%	2.070%
31	11.290	1303	1311	1325	rBV	199268	405084	24.52%	2.239%
32	12.124	1450	1453	1462	rBV4	3073	6644	0.40%	0.037%
33	12.518	1515	1520	1522	rBV	2875	3787	0.23%	0.021%
34	12.718	1548	1554	1561	rVV6	6274	11901	0.72%	0.066%

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35	13.223	1629	1640	1645	rBV7	3408	9666	0.59%	0.053%
36	13.299	1648	1653	1657	rVB4	3638	6451	0.39%	0.036%
37	13.352	1657	1662	1664	rBV3	2545	3517	0.21%	0.019%
38	13.458	1673	1680	1684	rBV7	6512	11722	0.71%	0.065%
39	13.546	1688	1695	1700	rBV3	3302	6329	0.38%	0.035%
40	13.599	1701	1704	1708	rBV2	3421	4002	0.24%	0.022%
41	13.740	1721	1728	1734	rBV3	4223	8377	0.51%	0.046%
42	13.810	1738	1740	1745	rVB4	2907	4775	0.29%	0.026%
43	14.139	1789	1796	1807	rVB2	13868	27055	1.64%	0.150%
44	14.263	1813	1817	1821	rBV5	3010	5861	0.35%	0.032%
45	14.339	1821	1830	1834	rVV	571391	867641	52.53%	4.796%
46	14.386	1834	1838	1851	rVB	258224	392666	23.77%	2.170%
47	14.645	1875	1882	1894	rVB	603115	992680	60.10%	5.487%
48	14.745	1894	1899	1902	rBV5	1629	3086	0.19%	0.017%
49	14.803	1903	1909	1916	rVB4	11108	17946	1.09%	0.099%
50	14.868	1916	1920	1926	rBV4	2480	4953	0.30%	0.027%
51	14.950	1926	1934	1942	rBV3	306143	530540	32.12%	2.933%
52	15.150	1960	1968	1986	rBV2	179555	394988	23.91%	2.183%
53	15.303	1991	1994	1997	rVV5	4057	5915	0.36%	0.033%
54	15.356	1997	2003	2007	rVB5	4045	8486	0.51%	0.047%
55	15.409	2007	2012	2022	rVV7	5625	13665	0.83%	0.076%
56	15.485	2022	2025	2029	rVB4	3585	4927	0.30%	0.027%
57	15.708	2059	2063	2064	rBV3	4396	4233	0.26%	0.023%
58	15.749	2066	2070	2076	rVB	23334	28725	1.74%	0.159%
59	15.802	2076	2079	2084	rBV4	3654	4174	0.25%	0.023%
60	15.937	2094	2102	2110	rBV	811716	1271167	76.96%	7.026%
61	16.061	2115	2123	2131	rBV2	221116	350965	21.25%	1.940%
62	16.155	2132	2139	2148	rVB3	14392	43383	2.63%	0.240%
63	16.237	2152	2153	2158	rVB3	2302	3459	0.21%	0.019%
64	16.302	2161	2164	2170	rVB6	4607	7025	0.43%	0.039%
65	16.378	2172	2177	2179	rBV4	4212	5464	0.33%	0.030%
66	16.496	2196	2197	2203	rVB4	4280	5807	0.35%	0.032%
67	16.554	2203	2207	2211	rBV5	4390	5721	0.35%	0.032%
68	16.607	2211	2216	2219	rBV3	29326	44399	2.69%	0.245%
69	16.801	2243	2249	2254	rVB7	3624	7580	0.46%	0.042%
70	16.960	2271	2276	2279	rVB5	2656	4479	0.27%	0.025%
71	17.013	2282	2285	2288	rVB2	3583	3594	0.22%	0.020%

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72	17.071	2292	2295	2300	rVV6	3363	5655	0.34%	0.031%
73	17.118	2300	2303	2310	rVB6	5160	8607	0.52%	0.048%
74	17.189	2311	2315	2317	rBV3	3599	4360	0.26%	0.024%
75	17.406	2347	2352	2357	rBV2	18314	27228	1.65%	0.151%
76	17.459	2357	2361	2368	rVV6	12201	20083	1.22%	0.111%
77	17.565	2374	2379	2381	rBV6	3916	3488	0.21%	0.019%
78	17.700	2395	2402	2412	rBV2	417553	655788	39.70%	3.625%
79	17.800	2412	2419	2430	rBV	913382	1400210	84.77%	7.740%
80	17.964	2440	2447	2448	rVB5	2875	6028	0.36%	0.033%
81	17.982	2448	2450	2452	rBV3	3947	4222	0.26%	0.023%
82	18.064	2461	2464	2473	rVB8	4813	8795	0.53%	0.049%
83	18.147	2473	2478	2484	rBV4	12049	18925	1.15%	0.105%
84	18.252	2493	2496	2500	rBV5	3526	4176	0.25%	0.023%
85	18.323	2504	2508	2514	rVB5	4913	5661	0.34%	0.031%
86	18.546	2541	2546	2555	rBV2	118223	195011	11.81%	1.078%
87	18.828	2592	2594	2599	rBV6	5151	6066	0.37%	0.034%
88	19.568	2717	2720	2722	rBV4	3461	3989	0.24%	0.022%
89	19.709	2734	2744	2749	rBV3	16633	39860	2.41%	0.220%
90	19.803	2755	2760	2771	rBV3	51214	97335	5.89%	0.538%
91	19.962	2783	2787	2792	rVB2	14840	23567	1.43%	0.130%
92	20.074	2799	2806	2815	rVB	1093866	1651764	100.00%	9.130%
93	21.595	3060	3065	3074	rBV4	66600	157911	9.56%	0.873%
94	22.030	3131	3139	3148	rVB	462364	837497	50.70%	4.629%
95	24.445	3545	3550	3560	rVB4	35609	82610	5.00%	0.457%
96	24.756	3597	3603	3616	rVB2	58913	139158	8.42%	0.769%
97	25.297	3683	3695	3712	rBV2	514555	1651333	99.97%	9.128%
98	25.532	3720	3735	3749	rVB2	238996	852504	51.61%	4.712%
99	26.701	3927	3934	3943	rVB5	42993	148430	8.99%	0.820%
100	26.989	3974	3983	3997	rVB4	86242	311844	18.88%	1.724%

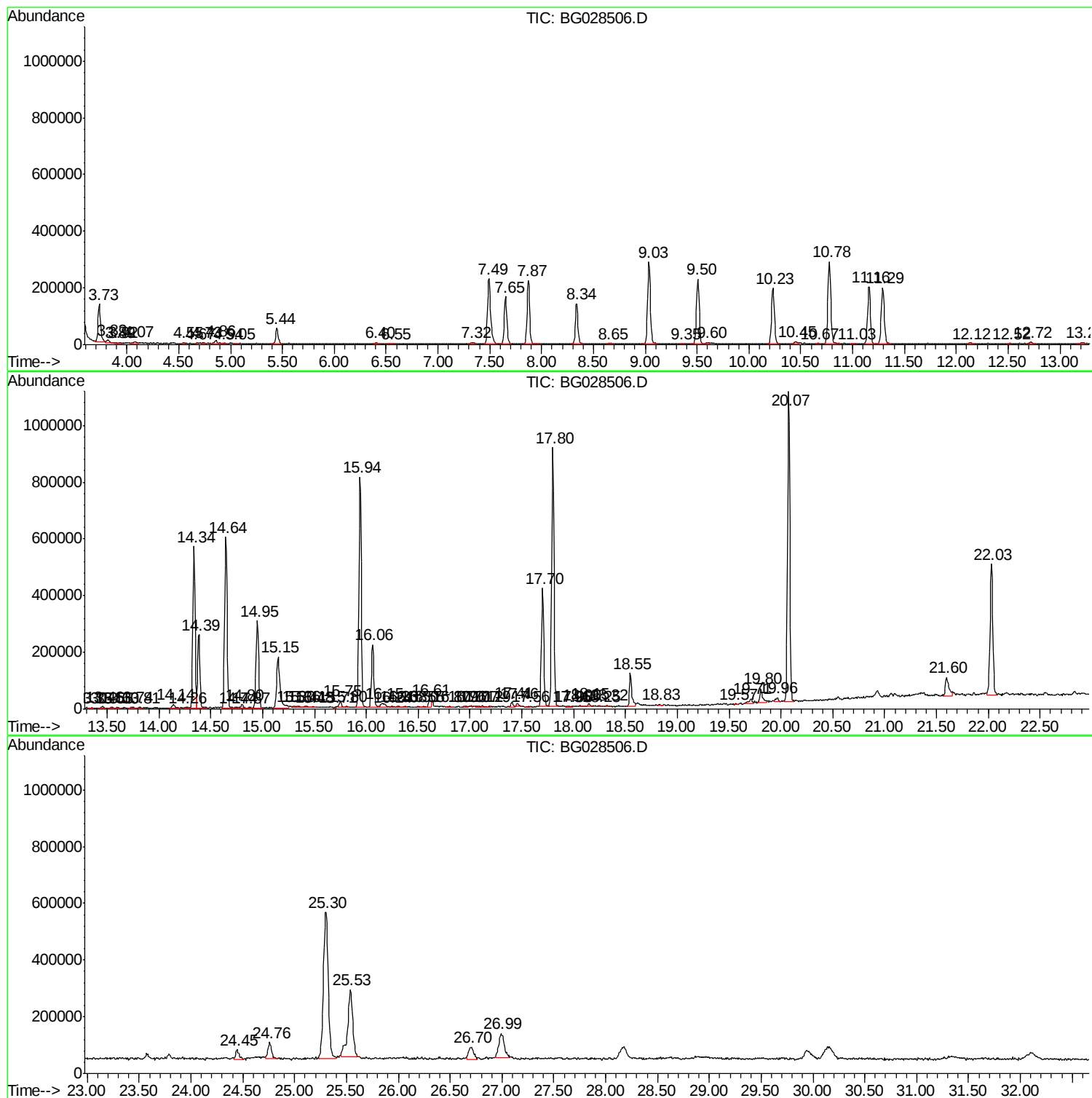
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

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



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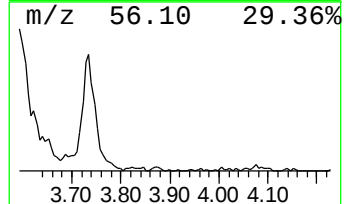
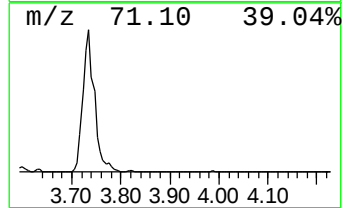
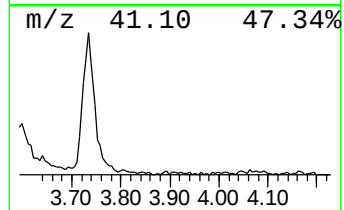
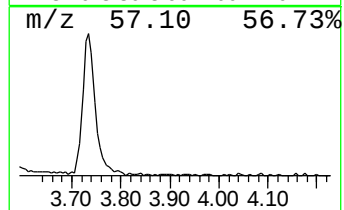
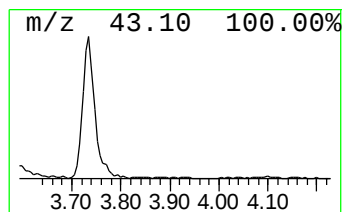
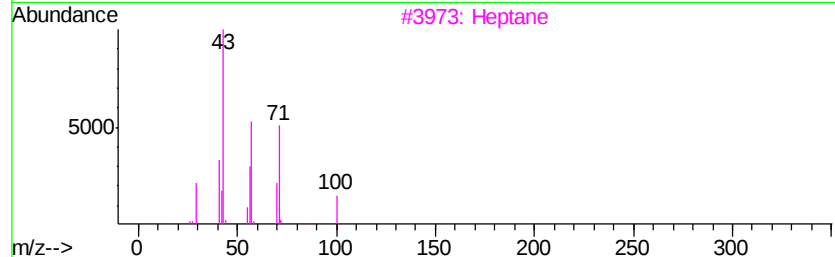
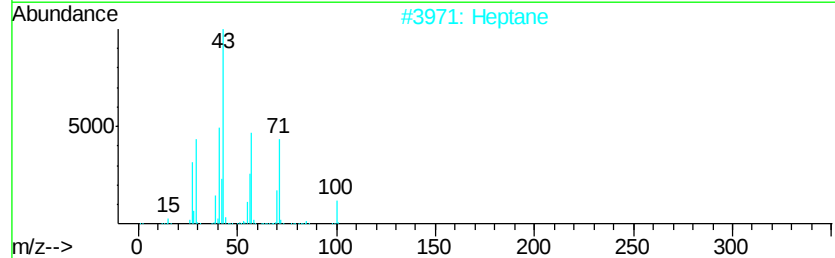
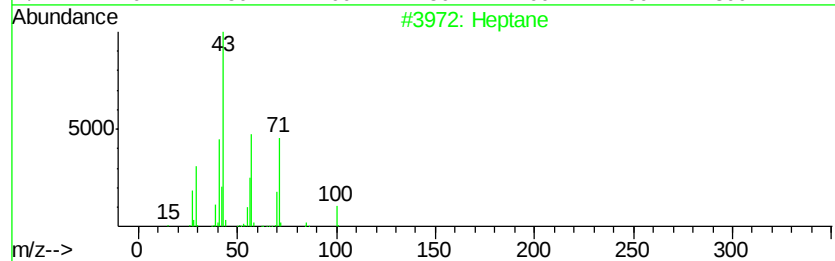
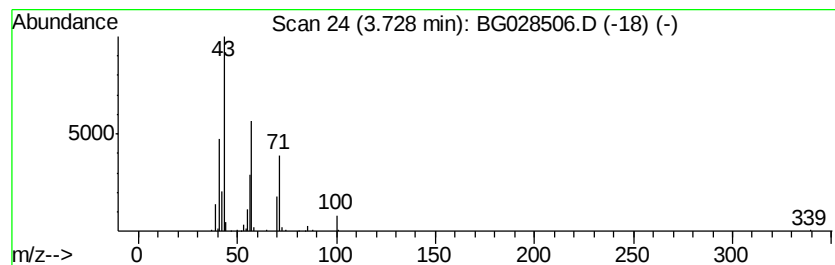
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.73	18.74 ng/ul	229706	1,4-Dichlorobenzene-d4	8.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane	100	C7H16	000142-82-5	95
2		Heptane	100	C7H16	000142-82-5	90
3		Heptane	100	C7H16	000142-82-5	86
4		Heptane	100	C7H16	000142-82-5	80
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	59



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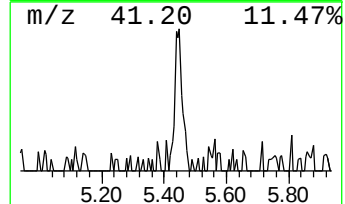
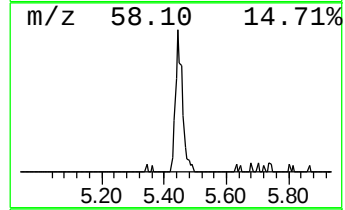
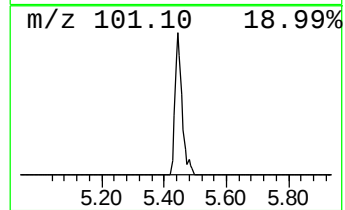
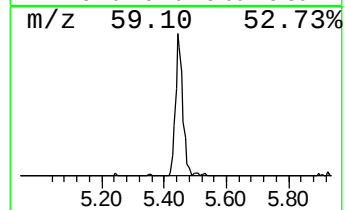
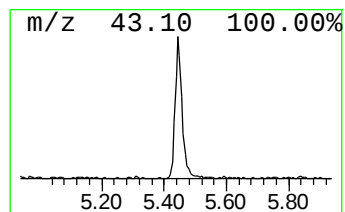
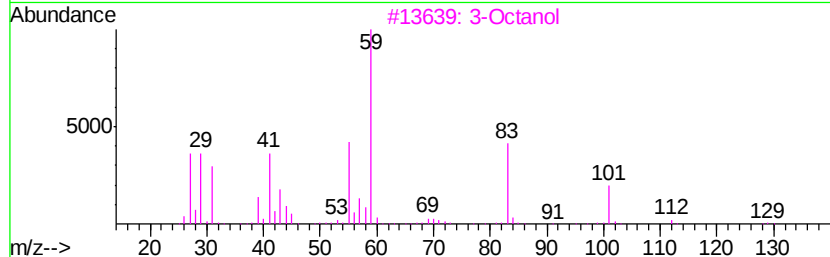
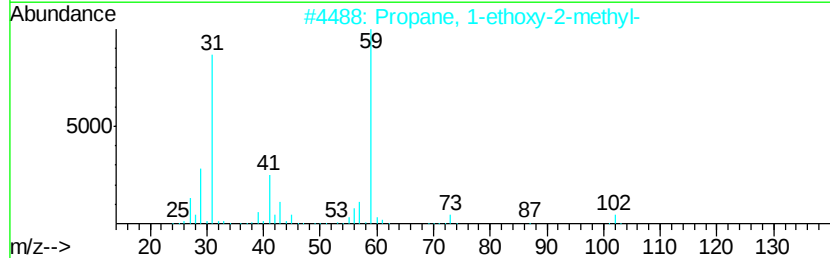
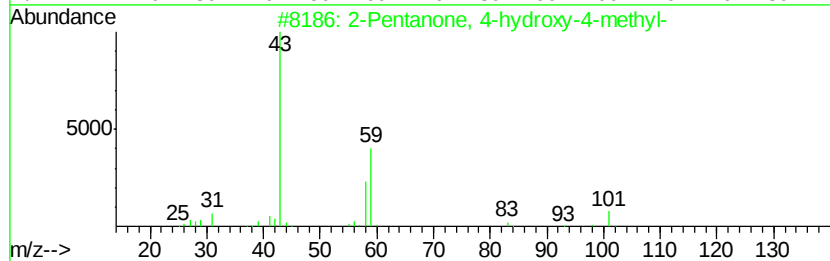
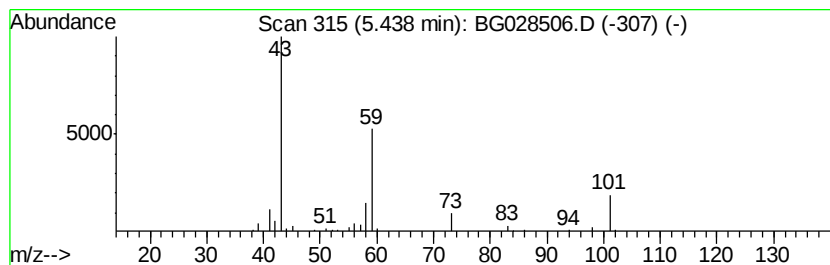
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.44	7.19 ng/ul	88125	1,4-Dichlorobenzene-d4	8.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	37
3		3-Octanol	130	C8H18O	000589-98-0	33
4		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32
5		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28



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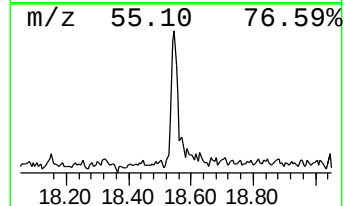
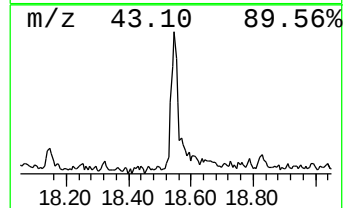
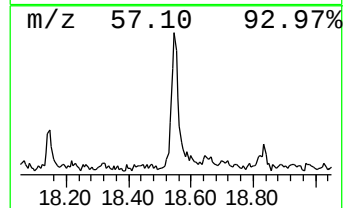
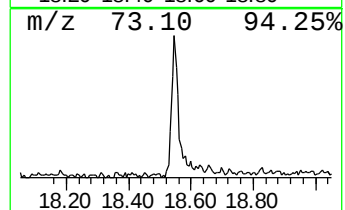
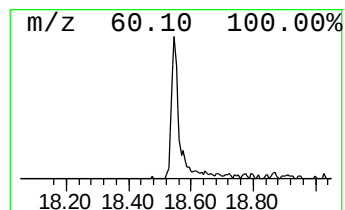
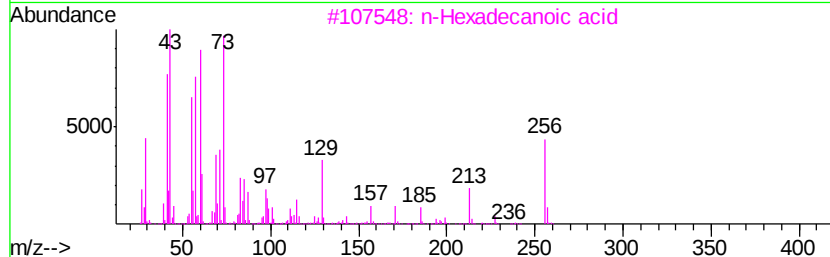
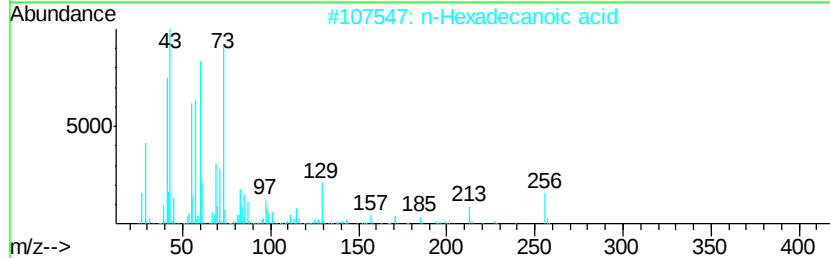
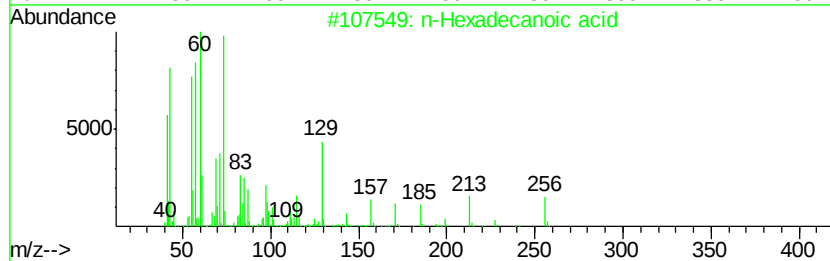
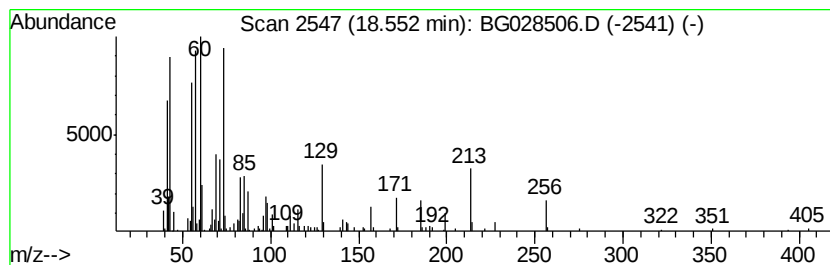
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TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	5.95 ng/ul	195011	Phenanthrene-d10	17.70

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	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90	
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76	
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76	



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082517\
Data File : BG028506.D
Acq On : 26 Aug 2017 00:59
Operator : SJ/JU
Sample : I4885-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B0AQ7

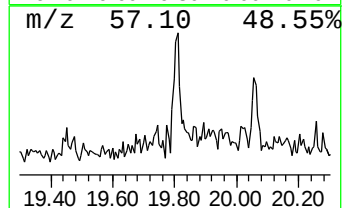
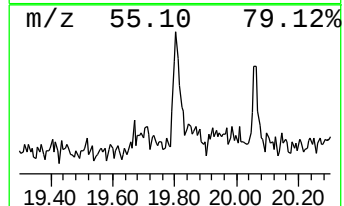
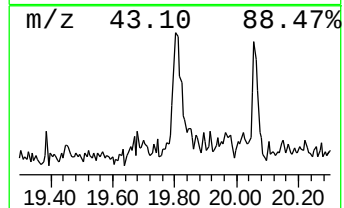
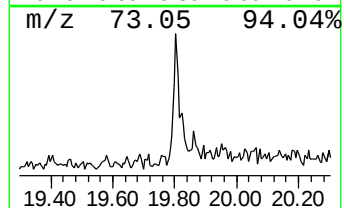
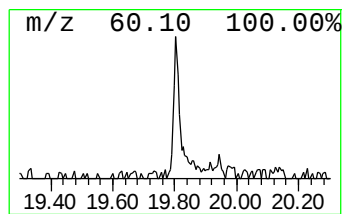
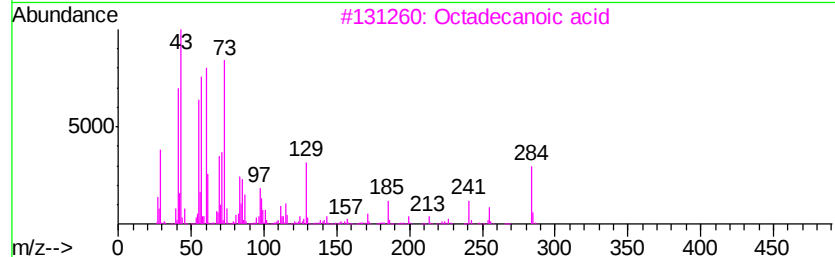
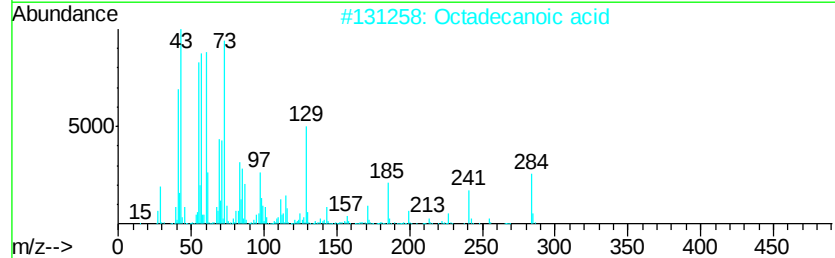
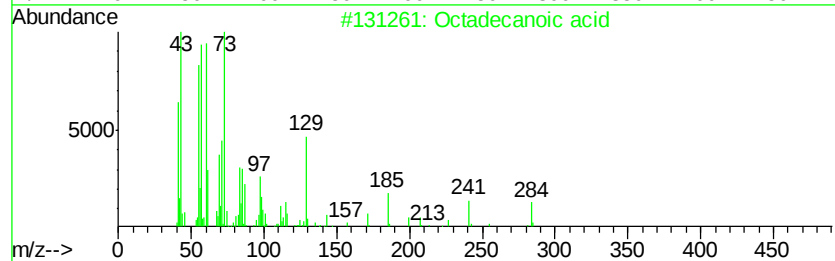
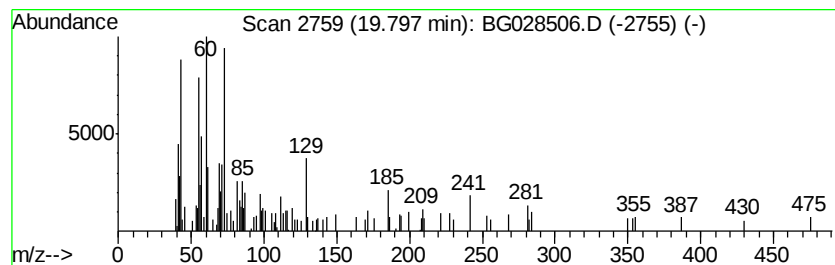
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.80	2.97 ng/ul	97335	Phenanthrene-d10		17.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Octadecanoic acid	284	C18H36O2	000057-11-4	91
3			Octadecanoic acid	284	C18H36O2	000057-11-4	90
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68



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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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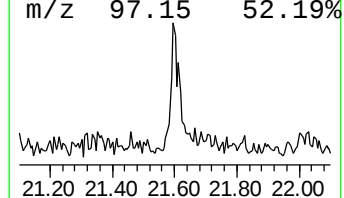
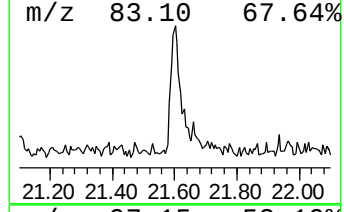
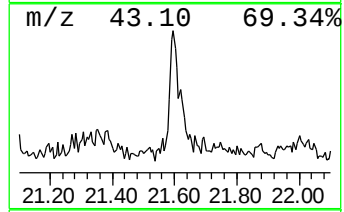
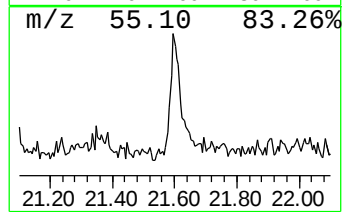
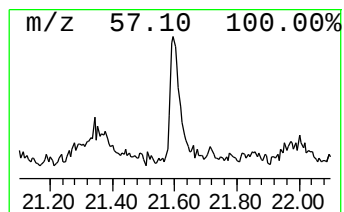
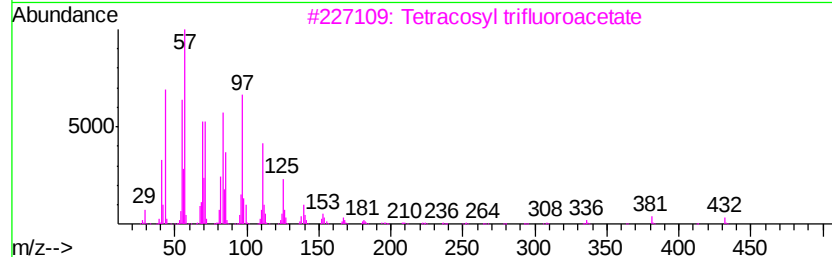
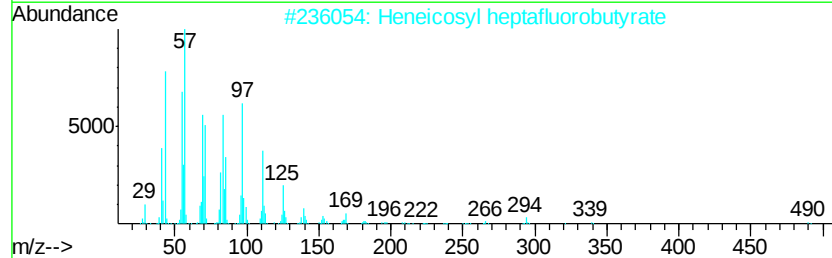
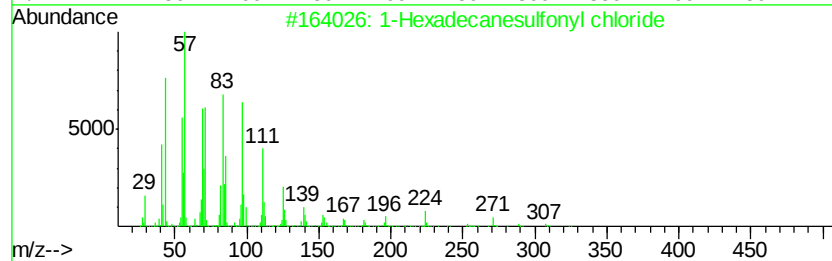
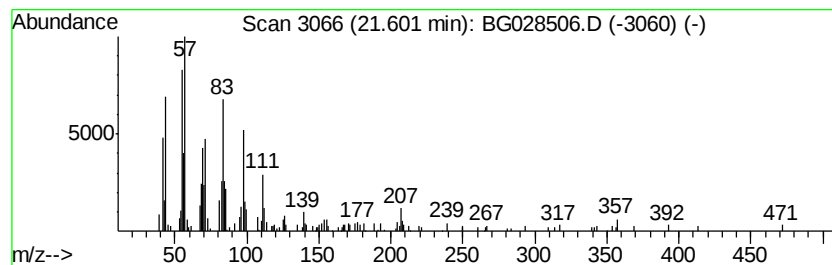
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1-Hexadecanesulfonyl chloride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.60	3.77 ng/ul	157911	Chrysene-d12	22.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	86
2		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	86
3		Tetracosyl trifluoroacetate	450	C26H49F3O2	1000351-76-4	86
4		1-Heptacosanol	396	C27H56O	002004-39-9	86
5		1-Hexacosanol	382	C26H54O	000506-52-5	68



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Operator : SJ/JU
Sample : I4885-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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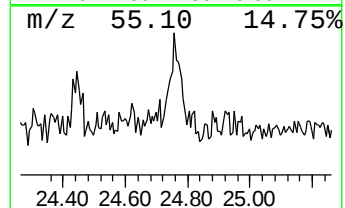
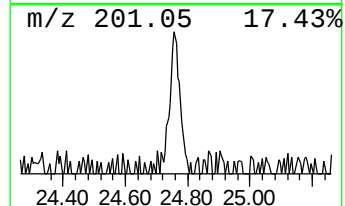
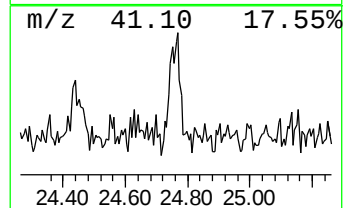
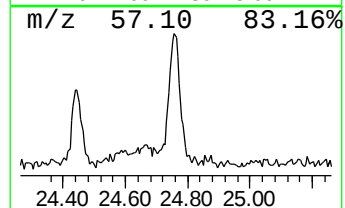
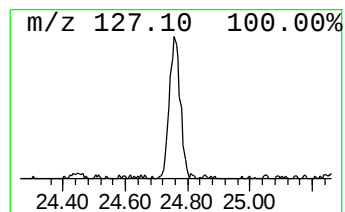
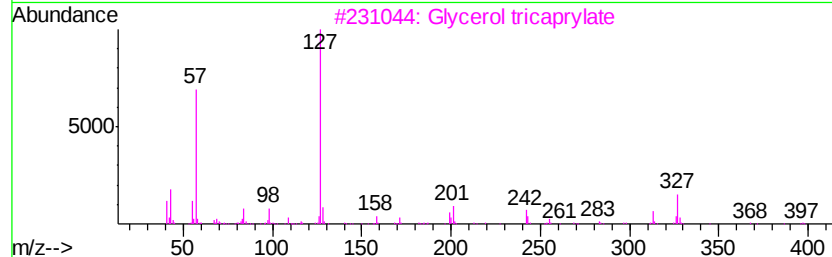
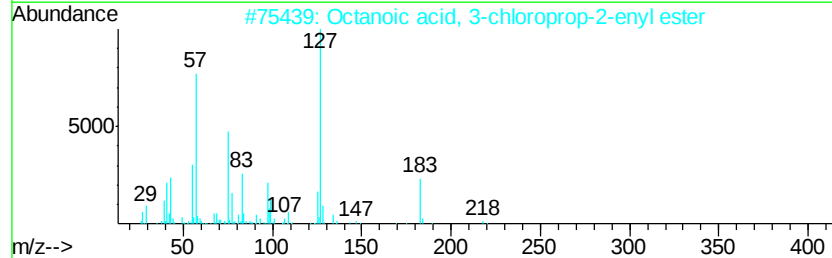
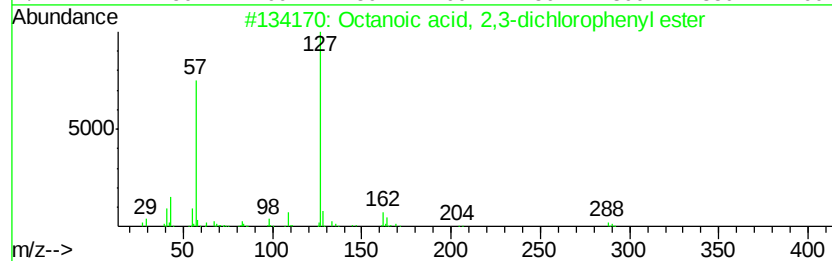
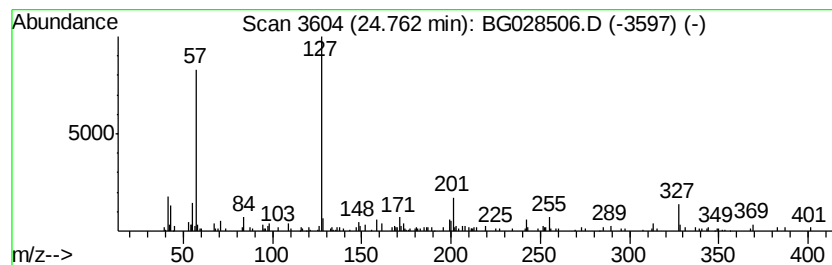
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Octanoic acid, 2,3-dichloro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.76	3.26 ng/ul	139158	Perylene-d12	25.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanoic acid, 2,3-dichloropheny...	288	C14H18Cl2O2	1000330-95-3	50
2		Octanoic acid, 3-chloroprop-2-en...	218	C11H19ClO2	1000299-35-0	50
3		Glycerol tricaprylate	470	C27H50O6	000538-23-8	50
4		Octanoic acid, 3,5-difluoropheny...	256	C14H18F2O2	1000293-68-2	47
5		2-Methyl-5-oxohexanethioic acid,...	216	C11H20O2S	1000186-90-2	47



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Sample : I4885-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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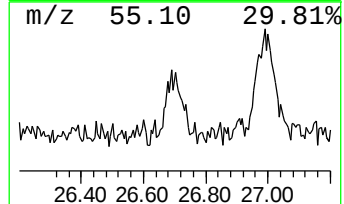
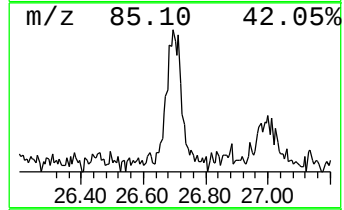
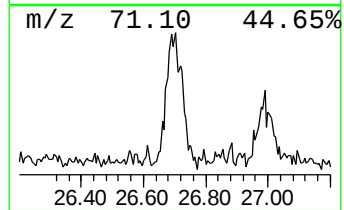
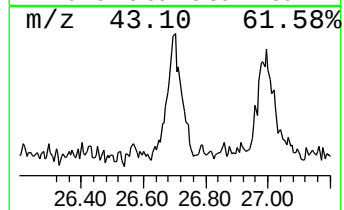
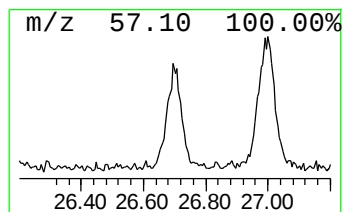
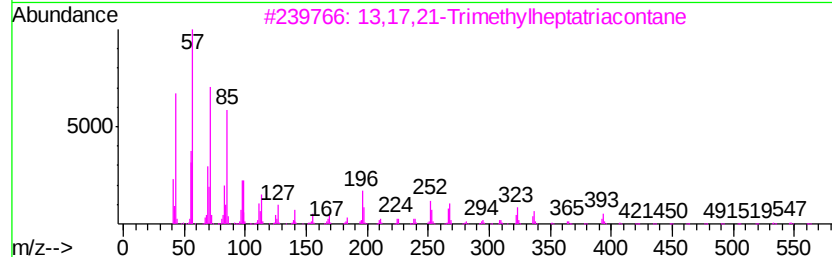
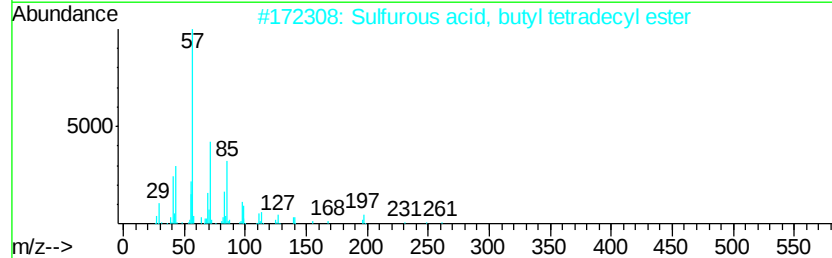
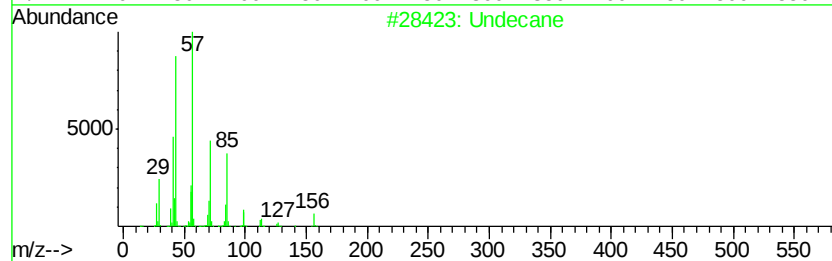
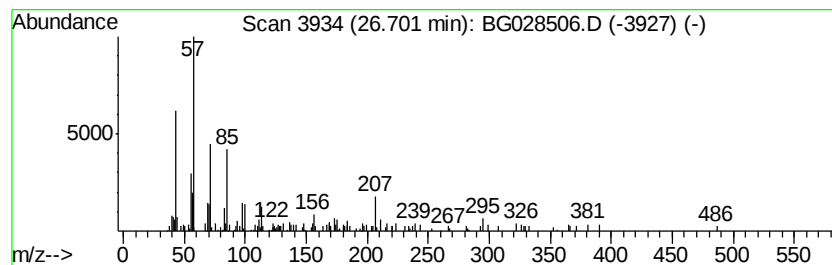
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.70	3.48 ng/ul	148430	Perylene-d12	25.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane	156	C11H24	001120-21-4	58
2		Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	58
3		13,17,21-Trimethylheptatriacontane	563	C40H82	058668-40-9	53
4		Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	50
5		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	50



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Misc :
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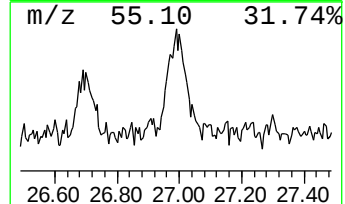
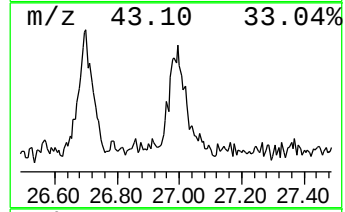
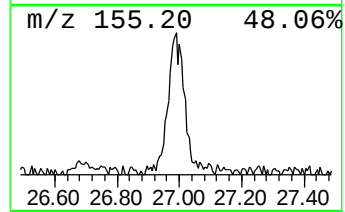
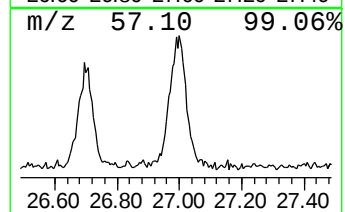
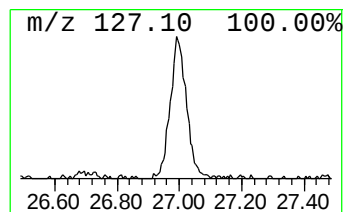
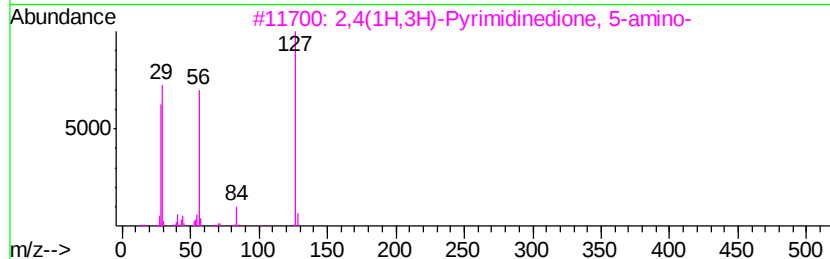
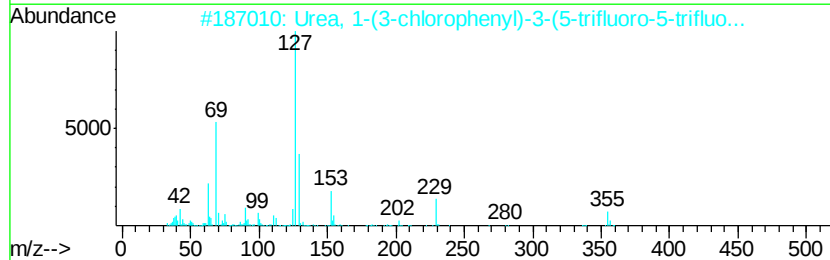
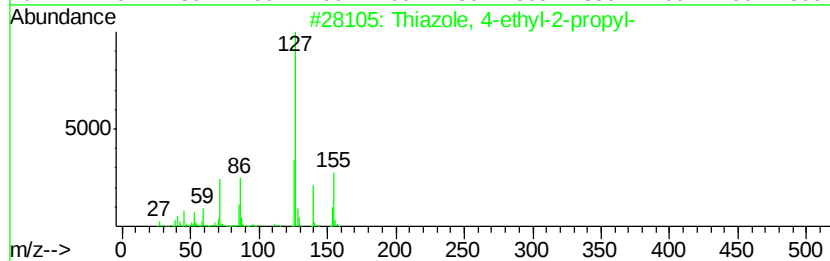
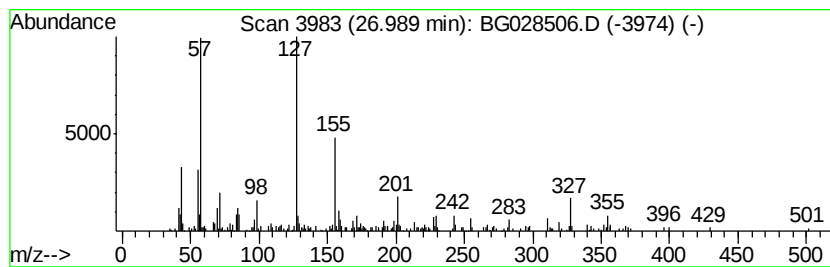
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.99	7.32 ng/ul	311844	Perylene-d12	25.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiazole, 4-ethyl-2-propyl-	155	C8H13NS	041981-68-4	42
2		Urea, 1-(3-chlorophenyl)-3-(5-tr...	355	C11H6ClF4N3O2S	1000270-41-1	37
3		2,4(1H,3H)-Pyrimidinedione, 5-am...	127	C4H5N3O2	000932-52-5	35
4		2,3,4-Trimethyl-isoxazol-5(2H)-one	127	C6H9N02	007713-68-0	35
5		2,5-Difluorobenzyl alcohol, 1-me...	200	C11H14F2O	1000378-16-5	35



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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.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
(DEL) Alkane: Str...	3.73	18.7	ng/ul	229706	1	8.34	245166	20.0
2-Pentanone, 4-hy...	5.44	7.2	ng/ul	88125	1	8.34	245166	20.0
n-Hexadecanoic acid	18.55	6.0	ng/ul	195011	4	17.70	655788	20.0
Octadecanoic acid	19.80	3.0	ng/ul	97335	4	17.70	655788	20.0
1-Hexadecanesulfo...	21.60	3.8	ng/ul	157911	5	22.03	837497	20.0
Octanoic acid, 2,...	24.76	3.3	ng/ul	139158	6	25.53	852504	20.0
(DEL) Alkane: Str...	26.70	3.5	ng/ul	148430	6	25.53	852504	20.0
unknown-01	26.99	7.3	ng/ul	311844	6	25.53	852504	20.0