

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG080817\
 Data File : BG028213.D
 Acq On : 9 Aug 2017 6:16
 Operator : SJ/JU
 Sample : I4557-06
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0AC9

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	3.841	38	43	50	rBV4	10696	18676	0.81%	0.097%
2	4.176	97	100	106	rVB4	2336	3409	0.15%	0.018%
3	4.446	142	146	150	rBV4	3094	4840	0.21%	0.025%
4	4.575	162	168	172	rVB5	2203	5228	0.23%	0.027%
5	5.832	380	382	388	rBV6	3335	5647	0.24%	0.029%
6	5.885	388	391	399	rVB5	3442	7248	0.31%	0.038%
7	6.003	405	411	418	rBV3	7298	17163	0.74%	0.089%
8	6.402	470	479	494	rVB3	66475	132209	5.72%	0.689%
9	6.984	574	578	584	rVB4	2506	4844	0.21%	0.025%
10	7.431	647	654	659	rBV2	3017	5470	0.24%	0.029%
11	7.501	659	666	679	rVB2	52912	107844	4.67%	0.562%
12	7.666	688	694	707	rVB	147447	248087	10.74%	1.293%
13	7.765	707	711	718	rVB3	2672	4934	0.21%	0.026%
14	7.883	722	731	740	rBV	152831	283188	12.26%	1.476%
15	8.353	803	811	828	rBV2	138206	313016	13.55%	1.632%
16	8.641	855	860	863	rVB3	2653	4162	0.18%	0.022%
17	8.964	907	915	920	rBV3	2820	5624	0.24%	0.029%
18	9.046	920	929	939	rVV	150213	276374	11.97%	1.441%
19	9.111	939	940	946	rVB2	2415	3501	0.15%	0.018%
20	9.181	946	952	960	rBV4	7926	13823	0.60%	0.072%
21	9.446	990	997	1003	rBV2	44545	79573	3.44%	0.415%
22	9.522	1003	1010	1025	rVB	203517	413406	17.90%	2.155%
23	10.245	1125	1133	1145	rVB3	179924	340405	14.74%	1.774%
24	10.615	1193	1196	1201	rVB3	2065	4170	0.18%	0.022%
25	10.785	1216	1225	1241	rBV	242319	470618	20.37%	2.453%
26	10.932	1247	1250	1257	rVB5	3555	7022	0.30%	0.037%
27	11.015	1257	1264	1267	rVV5	2402	5521	0.24%	0.029%
28	11.073	1267	1274	1284	rVV2	18482	44833	1.94%	0.234%
29	11.173	1284	1291	1305	rVB	208167	398600	17.26%	2.078%
30	11.661	1367	1374	1382	rBV8	6891	18701	0.81%	0.097%
31	11.749	1382	1389	1394	rVB5	3261	7489	0.32%	0.039%
32	11.831	1397	1403	1412	rVB3	8489	16491	0.71%	0.086%
33	12.425	1498	1504	1515	rBV2	49806	100132	4.34%	0.522%
34	12.736	1552	1557	1563	rVB4	5916	9102	0.39%	0.047%

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35	12.859	1575	1578	1583	rVB	2234	3406	0.15%	0.018%
36	13.030	1602	1607	1610	rVB2	2550	4220	0.18%	0.022%
37	13.230	1635	1641	1650	rVB3	3874	6866	0.30%	0.036%
38	13.312	1650	1655	1667	rBV3	9113	18559	0.80%	0.097%
39	13.559	1692	1697	1707	rVB2	15496	25806	1.12%	0.135%
40	13.829	1737	1743	1746	rBV3	3837	4942	0.21%	0.026%
41	13.876	1746	1751	1761	rVB	45622	86659	3.75%	0.452%
42	14.234	1807	1812	1818	rVB5	2485	5179	0.22%	0.027%
43	14.352	1821	1832	1847	rBV	670534	1018553	44.10%	5.309%
44	14.657	1876	1884	1893	rBV	614880	1001823	43.37%	5.222%
45	14.804	1907	1909	1918	rVB5	3468	6372	0.28%	0.033%
46	14.963	1924	1936	1943	rBV2	390823	652184	28.24%	3.400%
47	15.022	1943	1946	1954	rVB5	9109	13594	0.59%	0.071%
48	15.151	1960	1968	1988	rBV3	59630	147751	6.40%	0.770%
49	15.521	2027	2031	2034	rBV3	3421	3772	0.16%	0.020%
50	15.615	2040	2047	2055	rVB2	17318	30805	1.33%	0.161%
51	15.727	2062	2066	2068	rBV2	13334	18432	0.80%	0.096%
52	15.950	2096	2104	2115	rBV	943702	1456513	63.06%	7.592%
53	16.062	2115	2123	2137	rBV	430976	674437	29.20%	3.516%
54	16.191	2140	2145	2152	rVB6	10704	15791	0.68%	0.082%
55	16.308	2158	2165	2172	rBV5	5468	12424	0.54%	0.065%
56	16.726	2232	2236	2240	rBV	2341	3753	0.16%	0.020%
57	17.284	2326	2331	2338	rVB5	4912	7253	0.31%	0.038%
58	17.507	2364	2369	2376	rVB5	2486	4633	0.20%	0.024%
59	17.713	2395	2404	2412	rBV	620477	957171	41.44%	4.989%
60	17.813	2412	2421	2437	rVB	1203726	1908542	82.63%	9.949%
61	17.959	2443	2446	2451	rVB3	3926	5108	0.22%	0.027%
62	18.106	2463	2471	2473	rVB2	2370	4373	0.19%	0.023%
63	18.253	2492	2496	2502	rVB3	2254	4456	0.19%	0.023%
64	18.353	2507	2513	2521	rBV	369811	467202	20.23%	2.435%
65	18.523	2536	2542	2545	rBV4	5489	6935	0.30%	0.036%
66	18.559	2545	2548	2550	rBV2	2836	3580	0.15%	0.019%
67	18.641	2558	2562	2565	rVB	6074	7474	0.32%	0.039%
68	18.823	2587	2593	2601	rBV3	11170	15945	0.69%	0.083%
69	19.087	2632	2638	2642	rBV3	2854	4849	0.21%	0.025%
70	19.716	2739	2745	2754	rBV2	14025	22952	0.99%	0.120%
71	19.822	2758	2763	2771	rBV7	5475	13439	0.58%	0.070%

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72	19.969	2783	2788	2793	rVB2	12182	17412	0.75%	0.091%
73	20.086	2799	2808	2819	rBV	1581292	2309827	100.00%	12.040%
74	20.785	2924	2927	2930	rBV4	3652	4293	0.19%	0.022%
75	21.132	2982	2986	2988	rBV5	3727	4782	0.21%	0.025%
76	21.250	3004	3006	3011	rVB4	3300	4925	0.21%	0.026%
77	21.391	3022	3030	3031	rBV7	10326	19154	0.83%	0.100%
78	22.043	3133	3141	3151	rBV	625516	1115054	48.27%	5.812%
79	22.125	3153	3155	3159	rBV5	4404	4099	0.18%	0.021%
80	22.419	3203	3205	3209	rVB5	3979	3901	0.17%	0.020%
81	22.454	3209	3211	3219	rVB6	3014	5385	0.23%	0.028%
82	22.648	3241	3244	3249	rVB4	2227	3983	0.17%	0.021%
83	22.842	3273	3277	3286	rVB9	4993	11113	0.48%	0.058%
84	23.147	3326	3329	3333	rBV6	3205	4618	0.20%	0.024%
85	23.594	3400	3405	3412	rBV5	14723	28572	1.24%	0.149%
86	24.469	3546	3554	3561	rBV4	20684	46521	2.01%	0.242%
87	24.593	3572	3575	3576	rBV3	4852	4670	0.20%	0.024%
88	24.728	3596	3598	3608	rVB8	8566	16150	0.70%	0.084%
89	24.945	3633	3635	3638	rBV4	3635	4186	0.18%	0.022%
90	25.310	3683	3697	3715	rVB2	685940	2081519	90.12%	10.850%
91	25.545	3719	3737	3751	rBV	330683	1132563	49.03%	5.904%
92	26.726	3929	3938	3954	rVB5	29179	98236	4.25%	0.512%
93	27.060	3992	3995	4000	rBV6	4102	6414	0.28%	0.033%
94	27.413	4054	4055	4058	rBV3	3687	3371	0.15%	0.018%
95	28.206	4179	4190	4201	rVB5	26566	93464	4.05%	0.487%
96	28.958	4313	4318	4320	rBV4	5590	7081	0.31%	0.037%
97	29.334	4379	4382	4391	rVB7	3497	6674	0.29%	0.035%
98	29.975	4483	4491	4492	rBV6	17987	32113	1.39%	0.167%
99	31.514	4750	4753	4755	rBV3	2760	3959	0.17%	0.021%
100	32.143	4848	4860	4874	rVB10	15719	82946	3.59%	0.432%

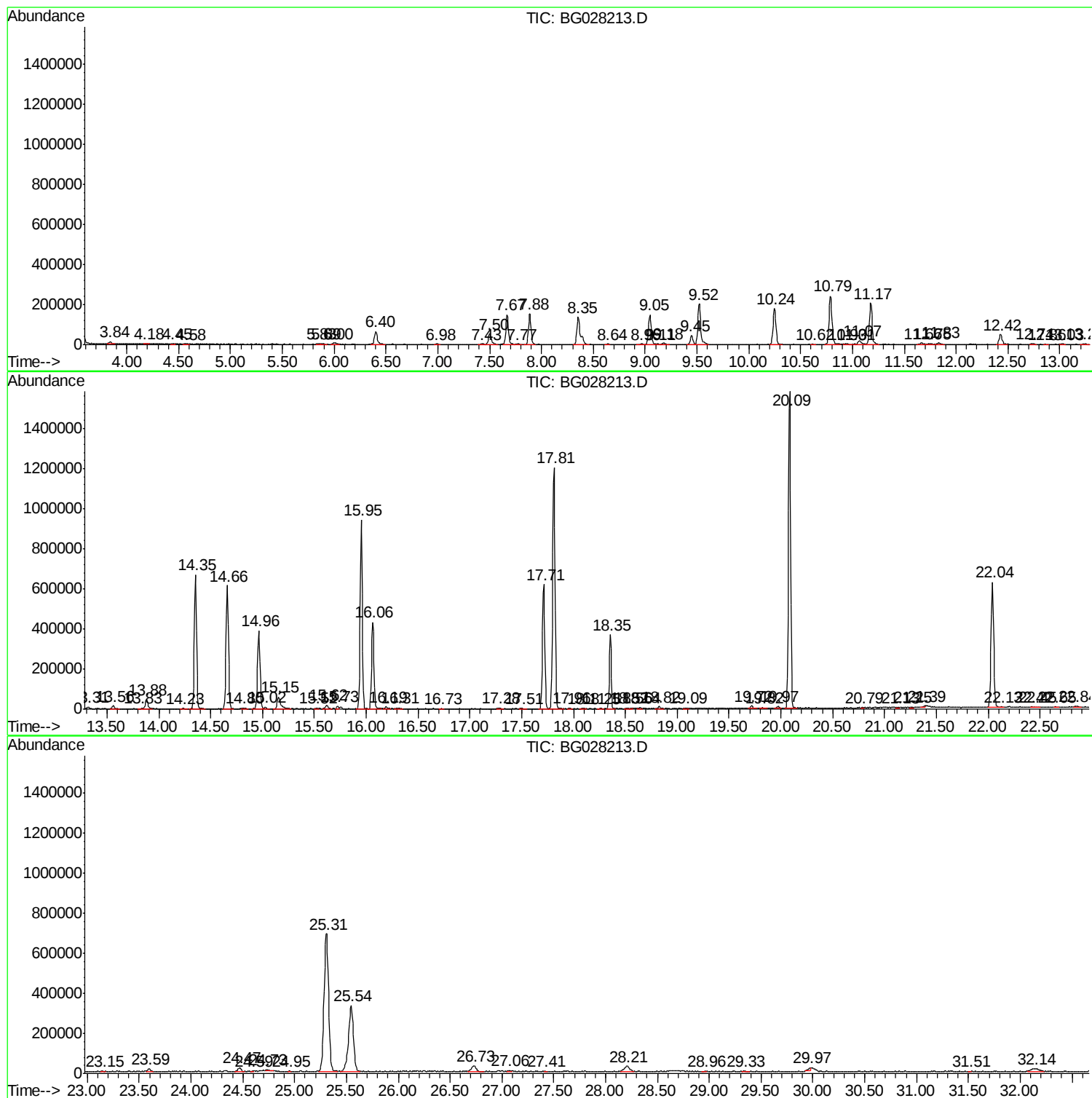
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

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



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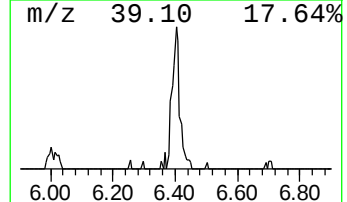
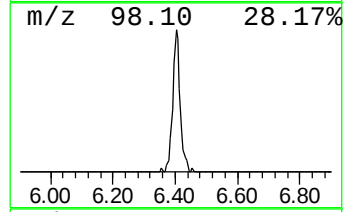
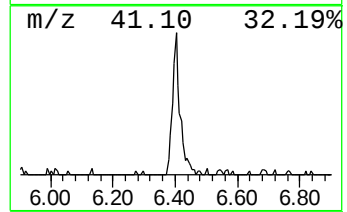
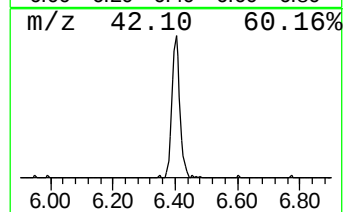
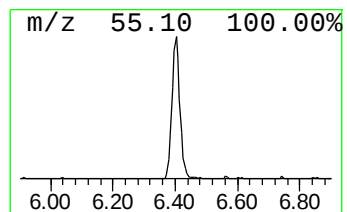
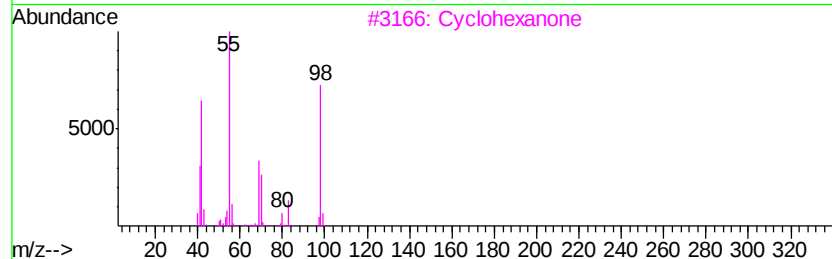
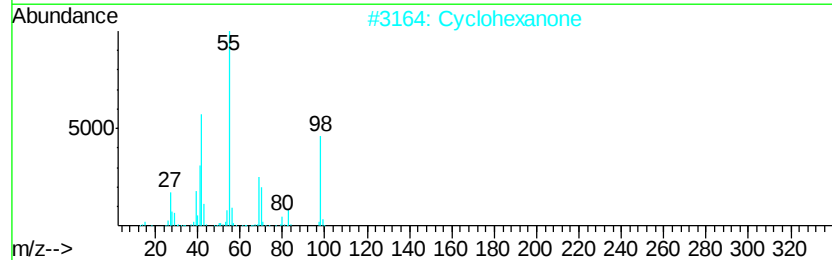
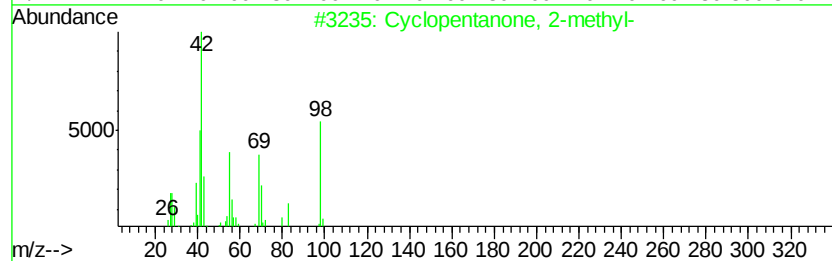
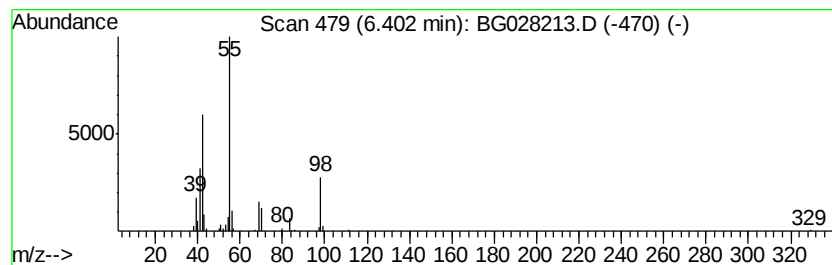
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Cyclopentanone, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	8.45 ng/ul	132209	1,4-Dichlorobenzene-d4	8.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	64
2			Cyclohexanone	98	C6H10O	000108-94-1	58
3			Cyclohexanone	98	C6H10O	000108-94-1	50
4			Diethylcyanamide	98	C5H10N2	000617-83-4	49
5			Cyclohexanone	98	C6H10O	000108-94-1	45



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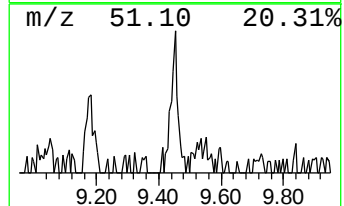
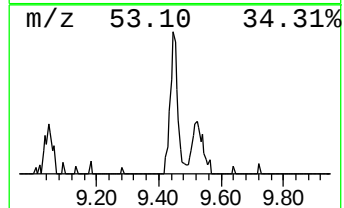
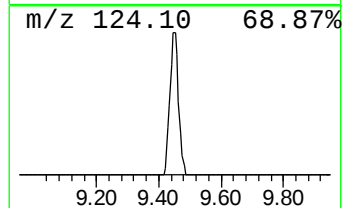
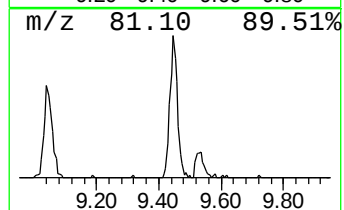
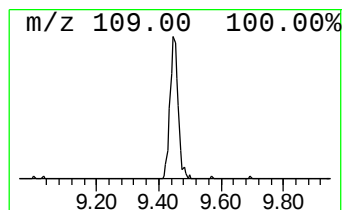
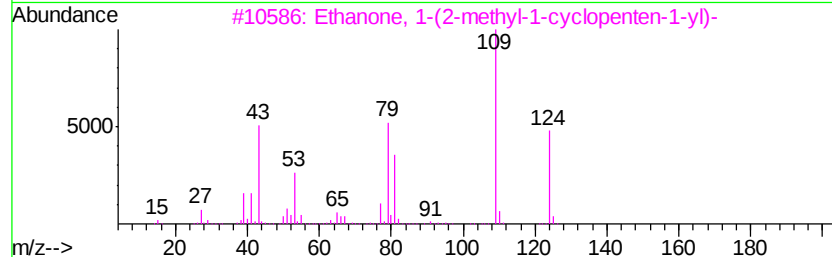
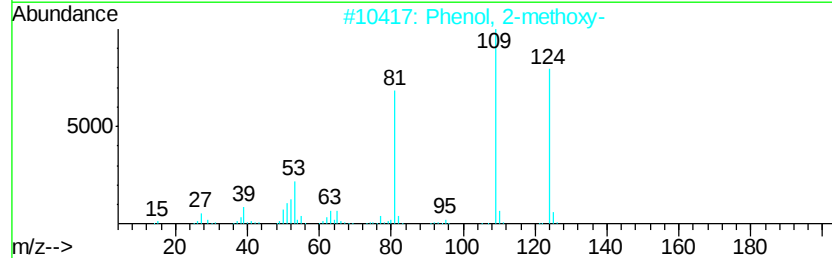
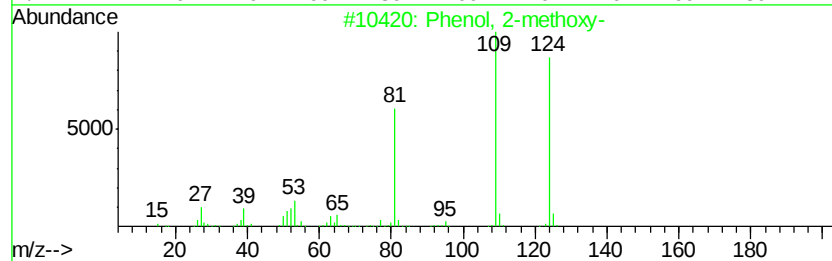
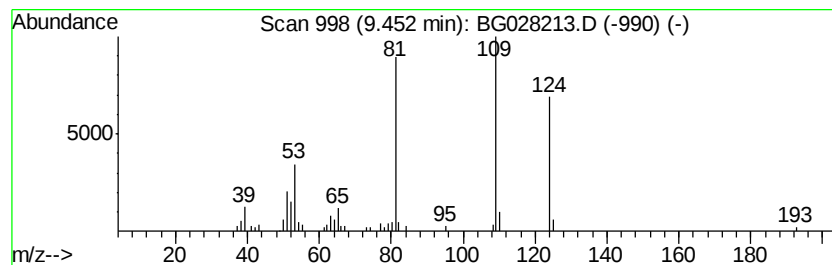
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Phenol, 2-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.45	5.08 ng/ul	79573	1,4-Dichlorobenzene-d4	8.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	87
2			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	78
3			Ethanone, 1-(2-methyl-1-cyclopent...	124	C8H12O	003168-90-9	64
4			Mequinol	124	C7H8O2	000150-76-5	50
5			5-Ethyl-2-furaldehyde	124	C7H8O2	023074-10-4	47



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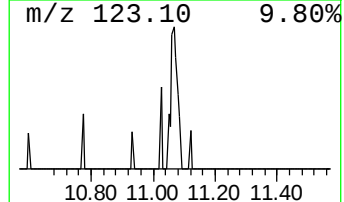
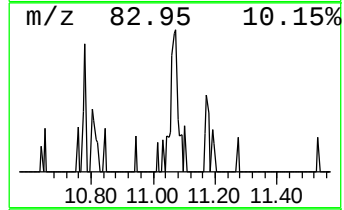
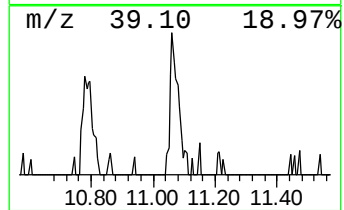
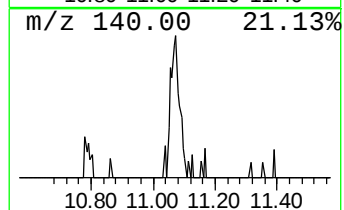
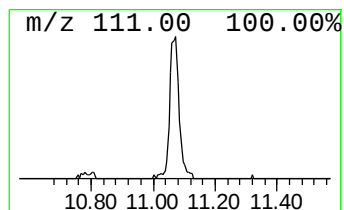
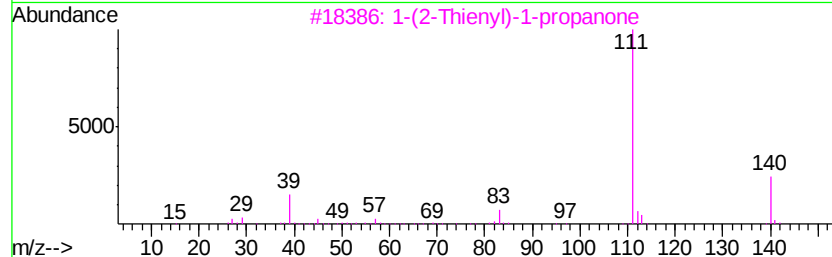
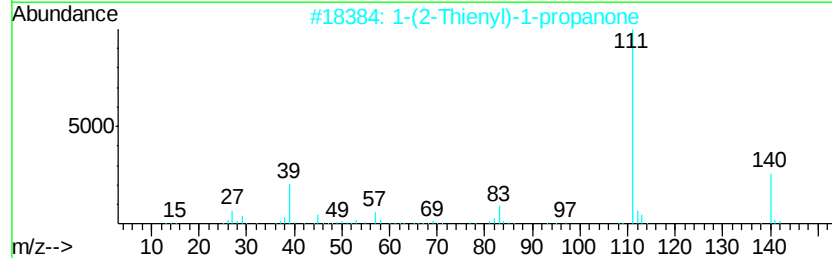
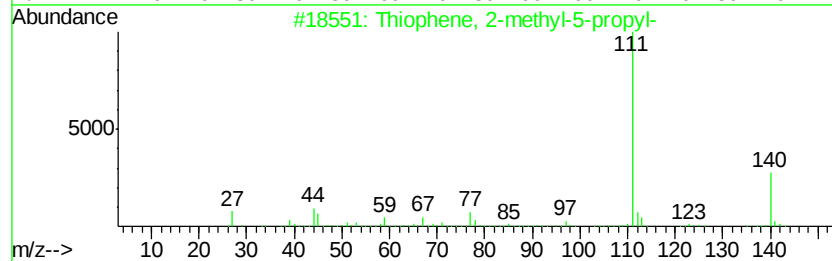
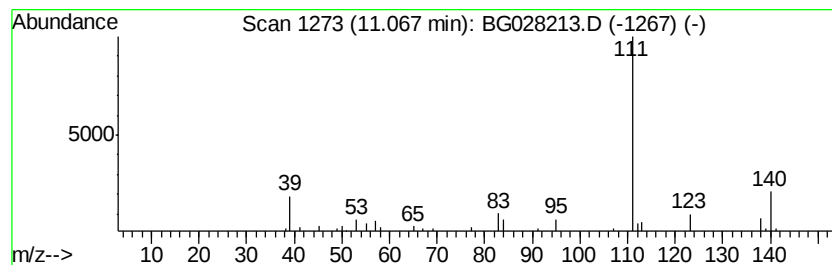
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Peak Number 3 Thiophene, 2-methyl-5-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.07	2.25 ng/ul	44833	Napthalene-d8	11.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene, 2-methyl-5-propyl-	140	C8H12S	033933-73-2	72
2		1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	64
3		1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	59
4		.gamma.-Chloro-2-butyrothienone	188	C8H9ClOS	043076-59-1	50
5		2-Thiophenecarboxylic acid, 4-fo...	262	C13H10O4S	1000338-38-0	50



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG080817\
Data File : BG028213.D
Acq On : 9 Aug 2017 6:16
Operator : SJ/JU
Sample : I4557-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AC9

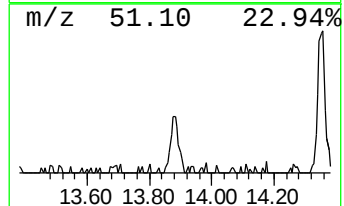
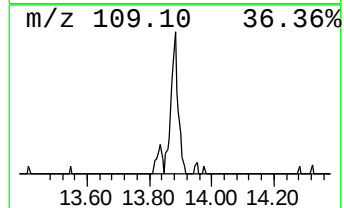
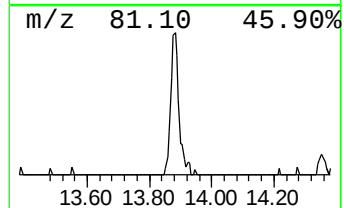
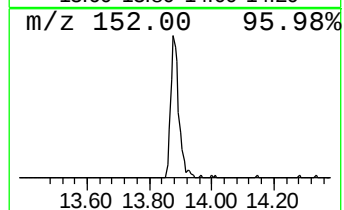
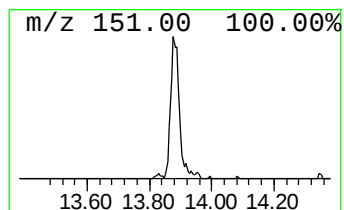
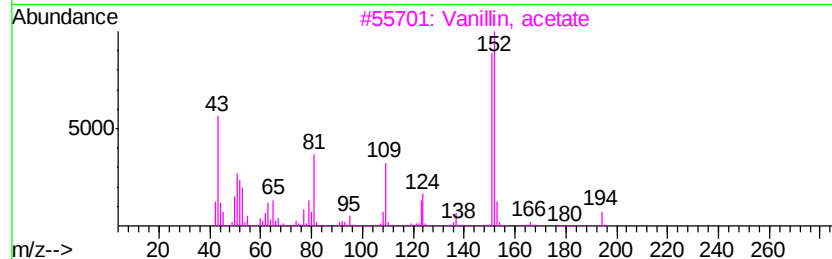
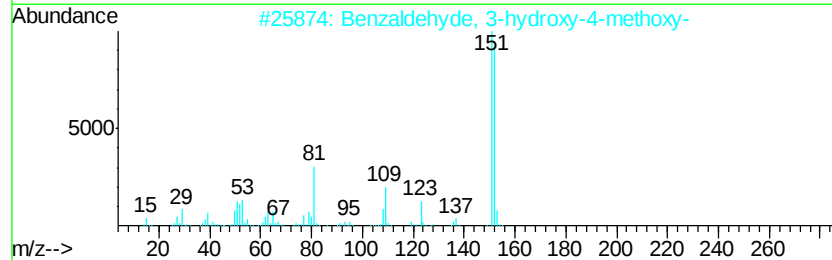
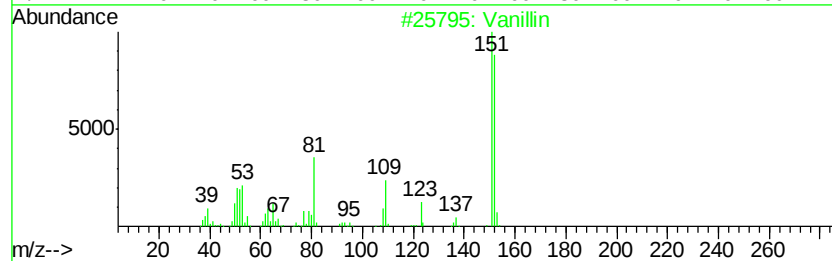
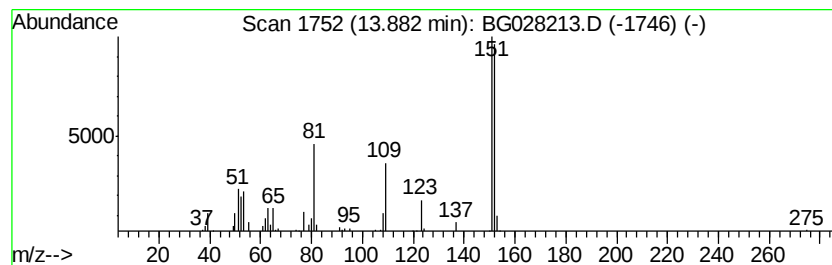
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Vanillin Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	2.66 ng/ul	86659	Acenaphthene-d10	14.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vanillin	152	C8H8O3	000121-33-5	97
2		Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	95
3		Vanillin, acetate	194	C10H10O4	000881-68-5	90
4		Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	83
5		Vanillin	152	C8H8O3	000121-33-5	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG080817\
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Sample : I4557-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AC9

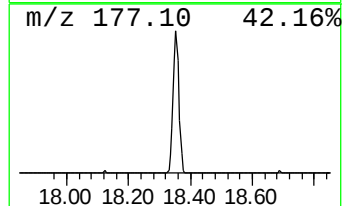
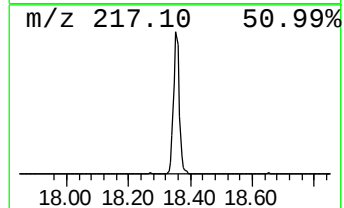
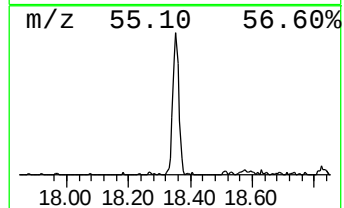
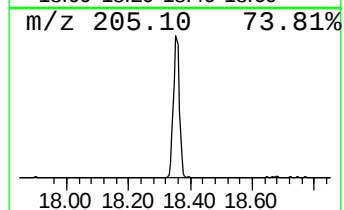
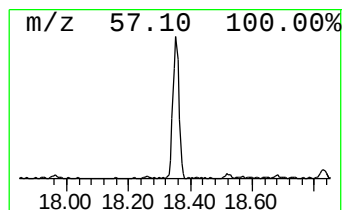
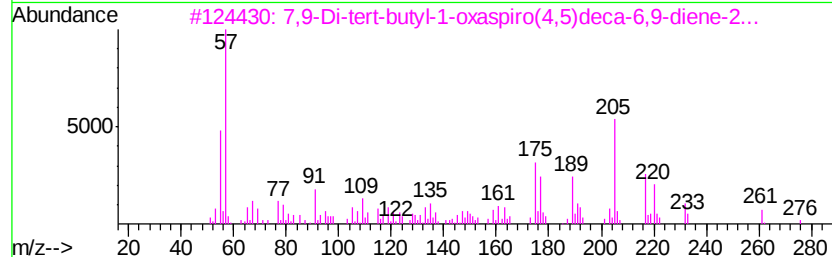
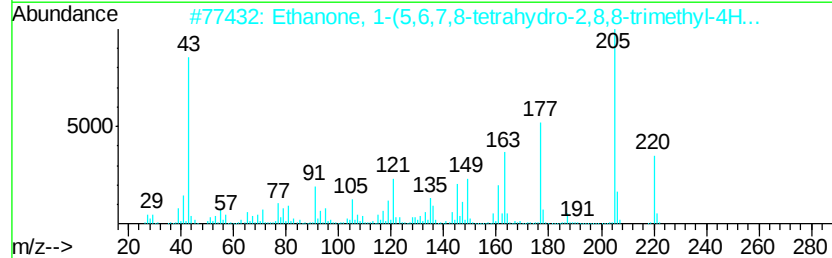
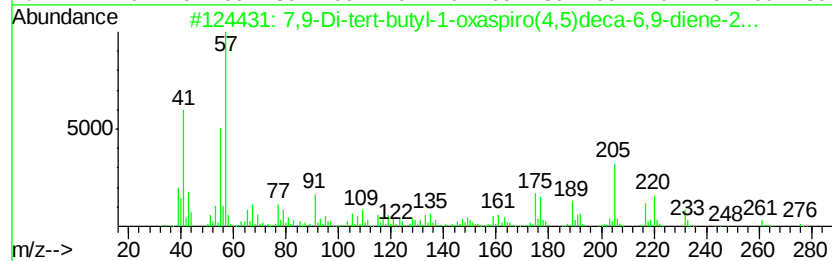
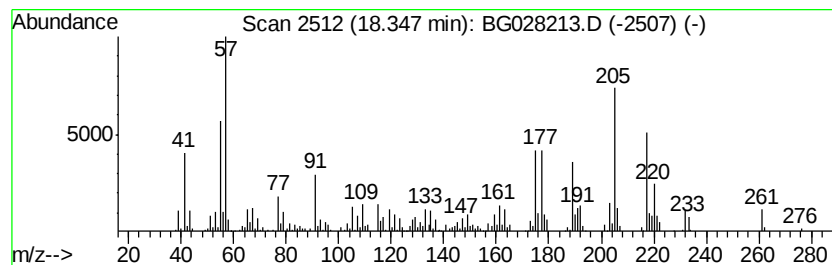
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	9.76 ng/ul	467202	Phenanthrene-d10	17.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	90		
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	64		
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	46		
4	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	42		
5	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	27		



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Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AC9

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
Cyclopentanone, 2...	6.40	8.4	ng/ul	132209	1	8.35	313016	20.0
Phenol, 2-methoxy-	9.45	5.1	ng/ul	79573	1	8.35	313016	20.0
Thiophene, 2-meth...	11.07	2.3	ng/ul	44833	2	11.17	398600	20.0
Vanillin	13.88	2.7	ng/ul	86659	3	14.96	652184	20.0
7,9-Di-tert-butyl...	18.35	9.8	ng/ul	467202	4	17.71	957171	20.0