

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091323\
 Data File : BG059054.D
 Acq On : 14 Sep 2023 00:54
 Operator : MA/JU
 Sample : 04280-01 10X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 JLAD0

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091023.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG059054.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.605	17	20	21	rBV3	14489	13890	0.28%	0.033%
2	3.634	21	25	29	rVV	96014	130989	2.65%	0.307%
3	3.963	77	81	87	rVB	44467	70849	1.43%	0.166%
4	4.046	89	95	107	rVB2	116272	237519	4.80%	0.557%
5	4.257	126	131	136	rBV2	23827	32518	0.66%	0.076%
6	4.339	142	145	150	rBV4	15827	21908	0.44%	0.051%
7	4.527	171	177	180	rBV5	12838	25748	0.52%	0.060%
8	4.627	188	194	201	rBV2	30265	56672	1.14%	0.133%
9	4.710	206	208	212	rBV4	10868	12157	0.25%	0.029%
10	4.798	220	223	224	rBV3	8906	10009	0.20%	0.023%
11	4.821	224	227	231	rVV	44456	55488	1.12%	0.130%
12	4.886	234	238	243	rVB2	32863	43361	0.88%	0.102%
13	5.279	301	305	310	rBV2	70333	95874	1.94%	0.225%
14	5.338	313	315	317	rVB3	9888	7571	0.15%	0.018%
15	5.561	352	353	359	rVB4	7350	9320	0.19%	0.022%
16	6.014	426	430	434	rBV4	10336	18769	0.38%	0.044%
17	6.208	459	463	466	rVB4	6736	10552	0.21%	0.025%
18	6.249	469	470	474	rBV4	9529	9079	0.18%	0.021%
19	6.314	477	481	482	rBV3	10078	9929	0.20%	0.023%
20	6.883	574	578	580	rVB5	15194	18724	0.38%	0.044%
21	7.019	596	601	603	rVB3	5051	7682	0.16%	0.018%
22	7.171	623	627	629	rBV4	6215	7887	0.16%	0.018%
23	7.265	642	643	648	rBV3	7049	8890	0.18%	0.021%
24	7.412	661	668	678	rVB3	124511	257989	5.21%	0.605%
25	7.618	695	703	709	rBV	361442	590236	11.92%	1.384%
26	7.812	727	736	744	rBV	362742	632661	12.78%	1.483%
27	8.000	766	768	770	rVB2	13296	10220	0.21%	0.024%
28	8.023	770	772	774	rBV3	9461	10195	0.21%	0.024%
29	8.299	813	819	827	rBV	337466	576522	11.64%	1.352%
30	8.499	850	853	856	rBV3	6358	7275	0.15%	0.017%
31	8.534	856	859	862	rBV3	7071	11029	0.22%	0.026%
32	8.611	870	872	874	rBV	9208	8381	0.17%	0.020%
33	8.822	906	908	911	rVB3	8096	7369	0.15%	0.017%
34	8.981	928	935	944	rBV2	378776	665813	13.45%	1.561%
35	9.140	957	962	967	rBV5	20715	39702	0.80%	0.093%
36	9.498	1013	1023	1031	rBV	493125	908080	18.34%	2.129%

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37	9.598	1035	1040	1042	rBV3	5690	9523	0.19%	0.022%
38	9.651	1044	1049	1052	rBV6	17287	25619	0.52%	0.060%
39	9.815	1076	1077	1081	rVB2	8184	7886	0.16%	0.018%
40	9.874	1083	1087	1088	rBV3	10343	12724	0.26%	0.030%
41	10.009	1109	1110	1112	rBV	9548	8601	0.17%	0.020%
42	10.150	1128	1134	1136	rBV4	24803	42175	0.85%	0.099%
43	10.215	1138	1145	1152	rVB2	422439	779854	15.75%	1.828%
44	10.514	1193	1196	1199	rVB5	6844	7811	0.16%	0.018%
45	10.579	1205	1207	1209	rBV3	7503	7712	0.16%	0.018%
46	10.738	1224	1234	1243	rBV	692519	1259724	25.44%	2.953%
47	11.143	1295	1303	1312	rBV	515567	924380	18.67%	2.167%
48	11.284	1320	1327	1338	rBV2	269087	528617	10.68%	1.239%
49	11.613	1376	1383	1388	rBV	404723	626344	12.65%	1.468%
50	11.672	1388	1393	1398	rVB	490085	750070	15.15%	1.759%
51	11.942	1434	1439	1444	rVB3	31164	53868	1.09%	0.126%
52	12.001	1446	1449	1450	rBV3	6306	7132	0.14%	0.017%
53	12.259	1491	1493	1496	rVB3	8444	7583	0.15%	0.018%
54	12.706	1564	1569	1573	rBV4	14854	25927	0.52%	0.061%
55	12.818	1586	1588	1592	rVB4	8408	10030	0.20%	0.024%
56	12.935	1604	1608	1612	rBV5	13019	20119	0.41%	0.047%
57	13.764	1743	1749	1755	rVB4	78200	129693	2.62%	0.304%
58	14.234	1827	1829	1833	rBV4	11457	17192	0.35%	0.040%
59	14.322	1838	1844	1850	rVV	1538856	2286341	46.17%	5.360%
60	14.369	1850	1852	1858	rVB2	51118	63738	1.29%	0.149%
61	14.633	1891	1897	1907	rBV	1552855	2442301	49.32%	5.726%
62	14.792	1919	1924	1930	rBV2	124195	188421	3.81%	0.442%
63	14.927	1941	1947	1956	rVB2	944294	1487293	30.04%	3.487%
64	15.021	1961	1963	1966	rVB3	11277	8319	0.17%	0.020%
65	15.097	1970	1976	1984	rBV	204363	324759	6.56%	0.761%
66	15.274	2004	2006	2008	rBV3	12362	10495	0.21%	0.025%
67	15.315	2011	2013	2017	rVB5	11701	12509	0.25%	0.029%
68	15.379	2021	2024	2026	rBV3	8873	9695	0.20%	0.023%
69	15.849	2101	2104	2107	rBV5	7921	11978	0.24%	0.028%
70	15.920	2109	2116	2123	rVV	2291694	3466988	70.02%	8.128%
71	16.020	2128	2133	2140	rVV	672733	999021	20.18%	2.342%
72	16.161	2153	2157	2163	rVB9	25715	51393	1.04%	0.120%
73	16.613	2227	2234	2239	rBV2	48867	88793	1.79%	0.208%
74	16.684	2242	2246	2247	rBV4	7683	8798	0.18%	0.021%
75	16.748	2255	2257	2263	rVB6	12967	19366	0.39%	0.045%
76	16.860	2274	2276	2278	rBV3	6837	7081	0.14%	0.017%

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77	17.013	2298	2302	2306	rBV7	9950	18637	0.38%	0.044%
78	17.189	2331	2332	2334	rBV2	7816	7258	0.15%	0.017%
79	17.348	2357	2359	2360	rVB2	12707	7927	0.16%	0.019%
80	17.436	2371	2374	2381	rBV8	11181	24265	0.49%	0.057%
81	17.512	2385	2387	2391	rVB4	7686	8018	0.16%	0.019%
82	17.683	2408	2416	2426	rBV	1396344	2142817	43.27%	5.024%
83	17.782	2426	2433	2440	rVV	2911715	4511571	91.11%	10.577%
84	18.305	2519	2522	2530	rVB10	16439	30563	0.62%	0.072%
85	18.452	2544	2547	2551	rVB5	19290	23594	0.48%	0.055%
86	18.499	2551	2555	2564	rBV2	108440	188030	3.80%	0.441%
87	18.628	2575	2577	2578	rVB2	16592	9857	0.20%	0.023%
88	18.646	2578	2580	2582	rBV3	15500	12783	0.26%	0.030%
89	18.728	2592	2594	2597	rVB4	10728	9077	0.18%	0.021%
90	18.770	2600	2601	2603	rBV2	11088	10345	0.21%	0.024%
91	18.881	2617	2620	2621	rBV3	11115	10269	0.21%	0.024%
92	19.052	2647	2649	2650	rBV2	14870	10305	0.21%	0.024%
93	19.492	2721	2724	2728	rVB5	52457	72116	1.46%	0.169%
94	19.616	2741	2745	2749	rBV6	54938	84072	1.70%	0.197%
95	19.680	2754	2756	2762	rVB2	43651	51794	1.05%	0.121%
96	19.762	2767	2770	2775	rVV7	45786	63964	1.29%	0.150%
97	20.056	2814	2820	2826	rBV	3332908	4951693	100.00%	11.609%
98	22.001	3145	3151	3158	rBV2	1153131	2093124	42.27%	4.907%
99	25.315	3705	3715	3727	rVB3	1560333	4781115	96.56%	11.209%
100	25.556	3748	3756	3766	rVB	682944	2139896	43.22%	5.017%

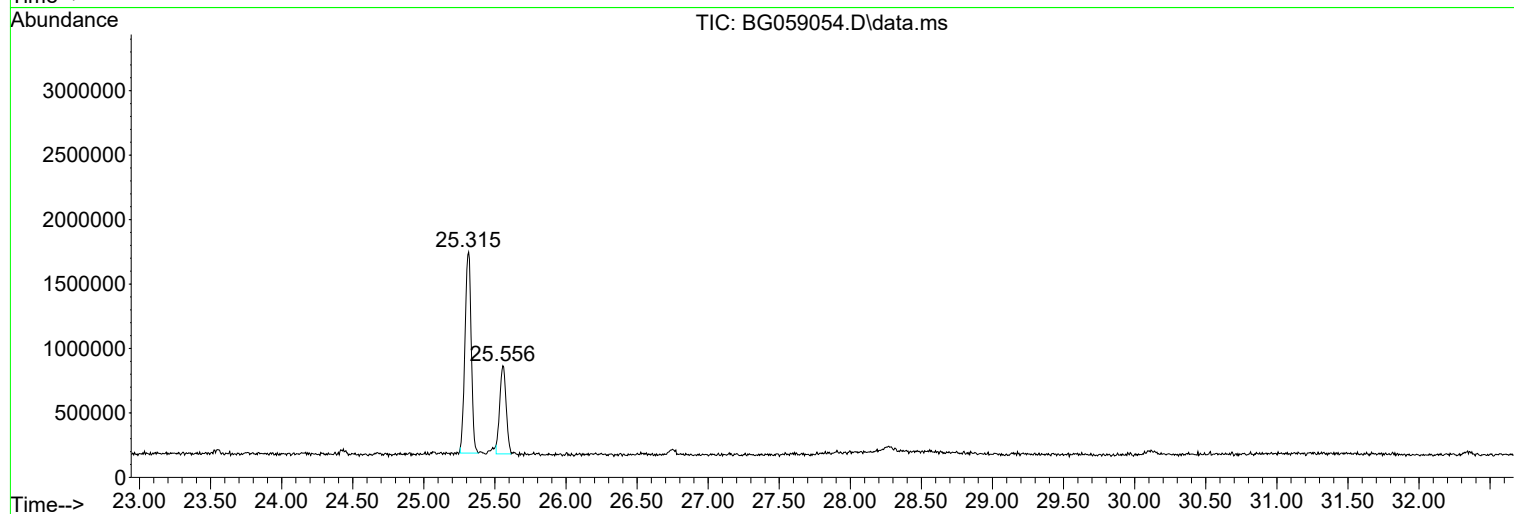
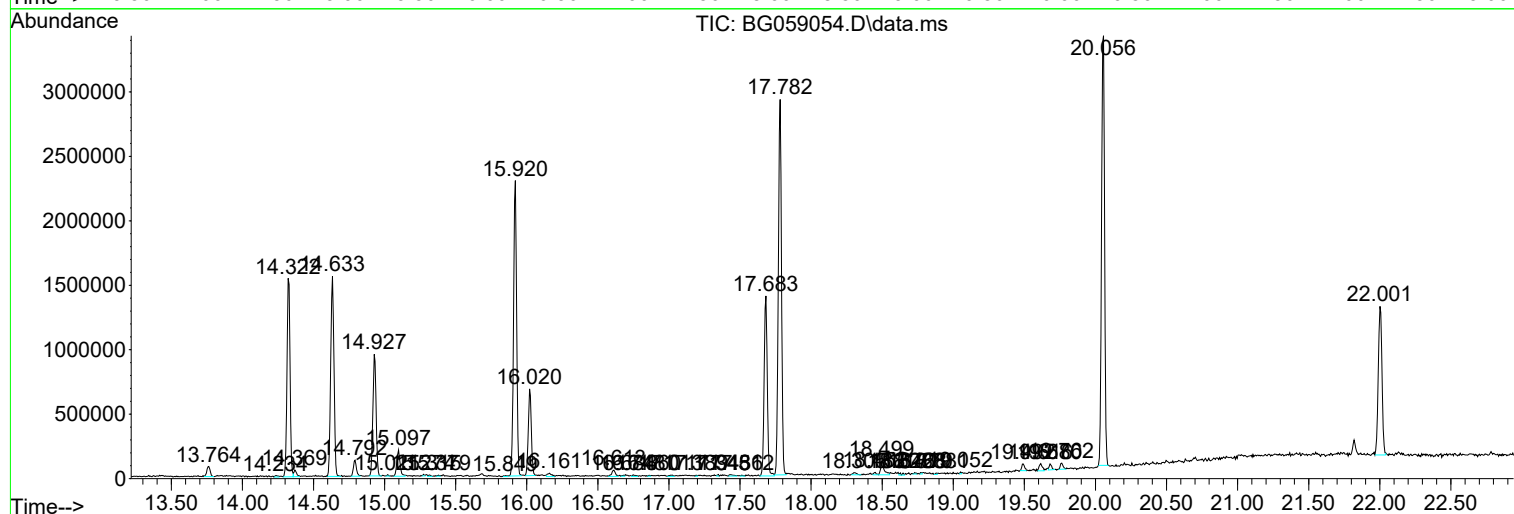
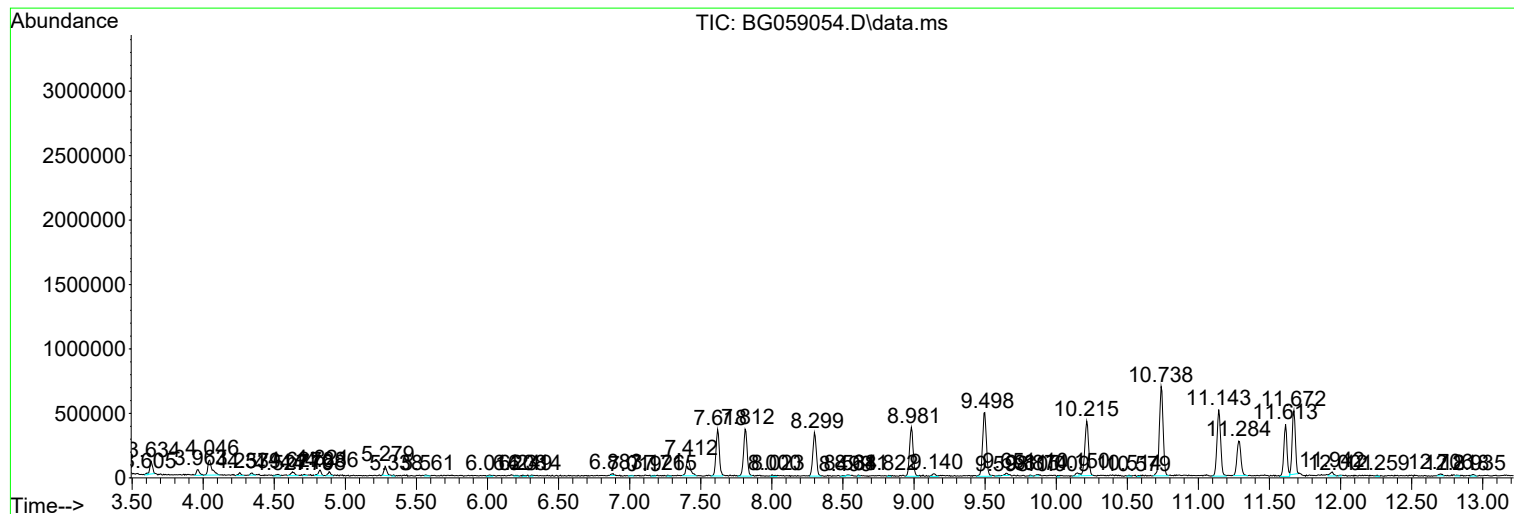
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091023.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P



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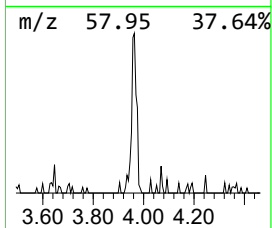
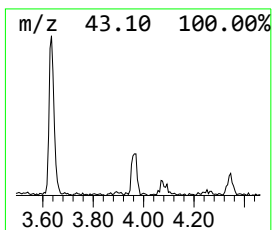
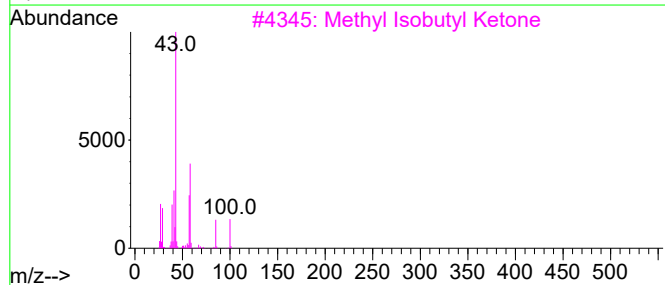
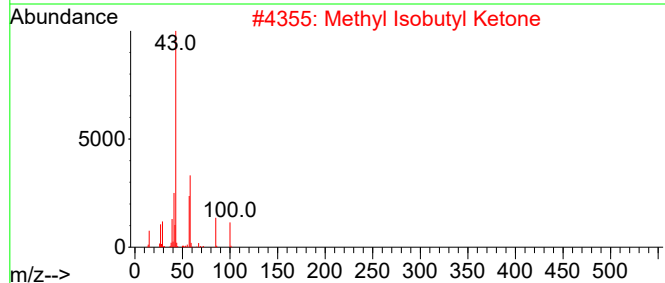
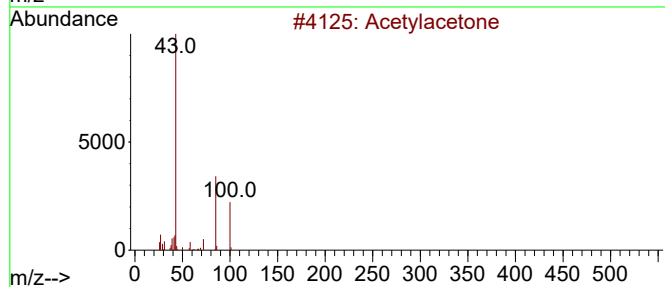
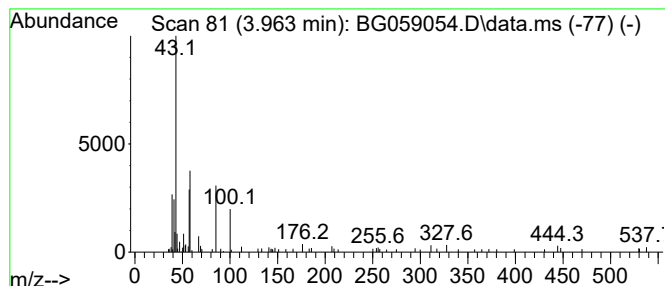
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091023.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetylacetone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.963	2.46 ng/ul	70849	1,4-Dichlorobenzene-d4	8.305

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetylacetone	100	C5H8O2	000123-54-6	52
2			Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	50
3			Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	50
4			Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	43
5			Acetylacetone	100	C5H8O2	000123-54-6	40



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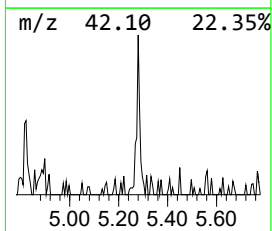
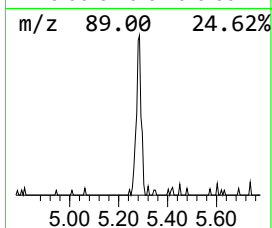
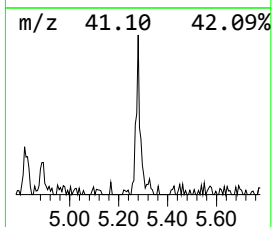
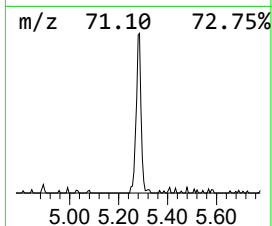
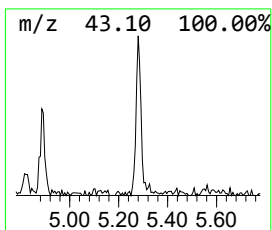
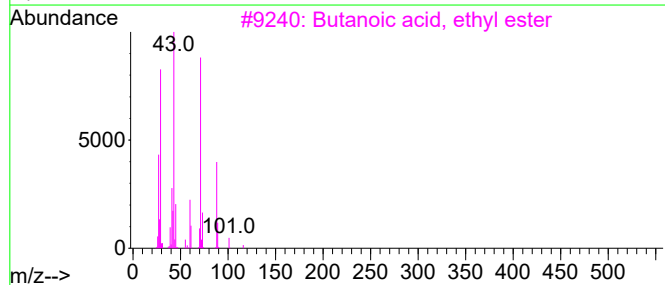
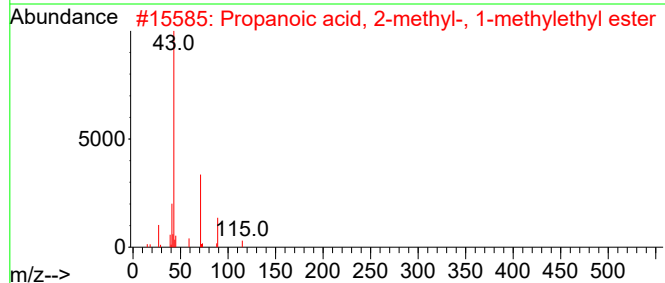
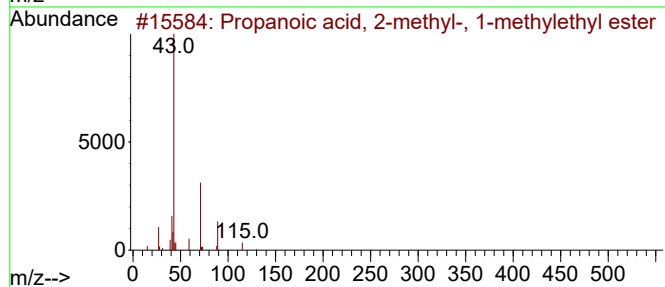
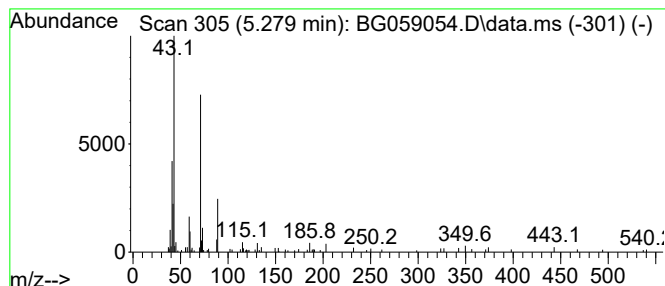
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091023.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.279	3.33 ng/ul	95874	1,4-Dichlorobenzene-d4	8.305

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	53
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	53
3			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	47
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	45
5			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	45



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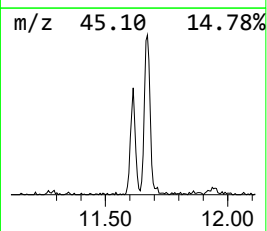
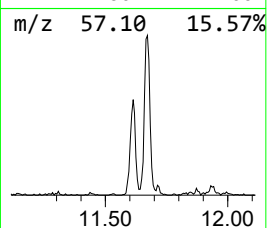
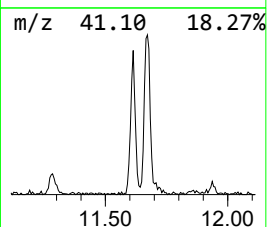
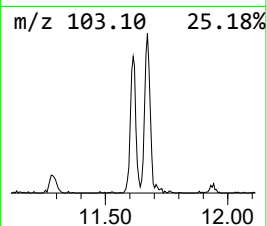
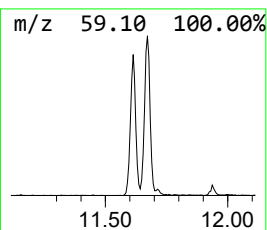
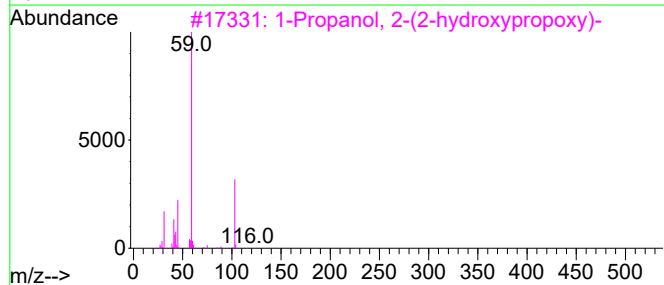
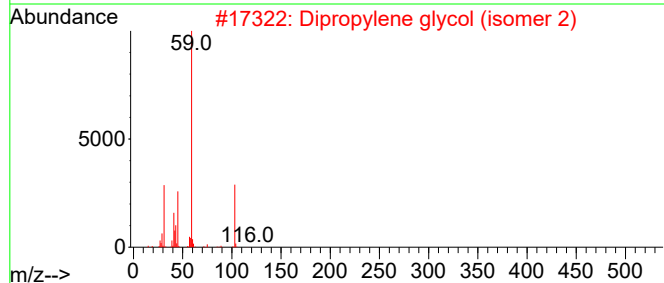
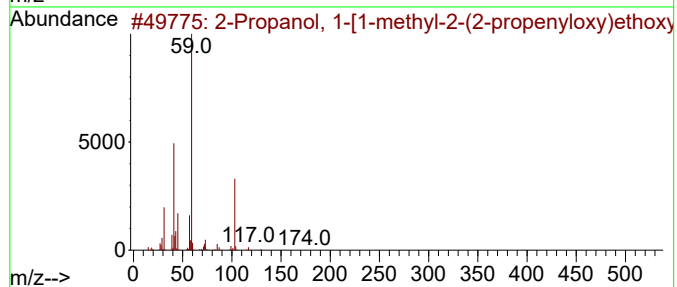
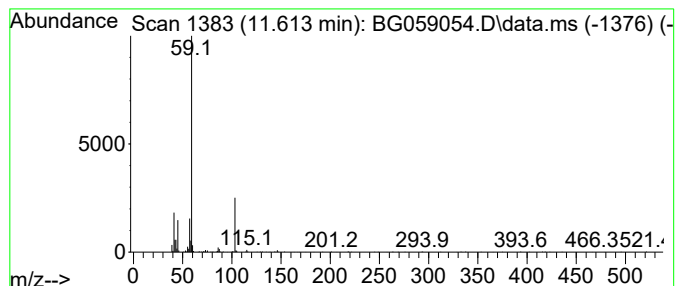
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091023.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.613	13.55 ng/ul	626344	Naphthalene-d8	11.143

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	83		
2	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	78		
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78		
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	78		
5	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	74		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091323\
Data File : BG059054.D
Acq On : 14 Sep 2023 00:54
Operator : MA/JU
Sample : 04280-01 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JLAD0

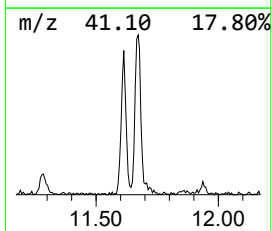
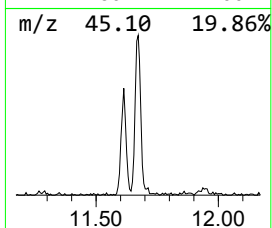
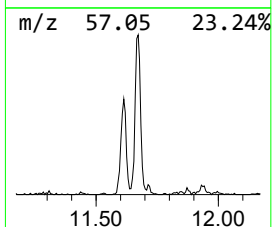
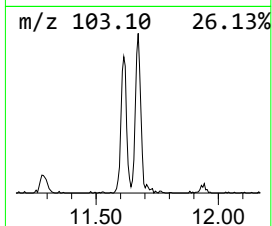
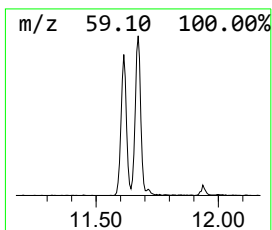
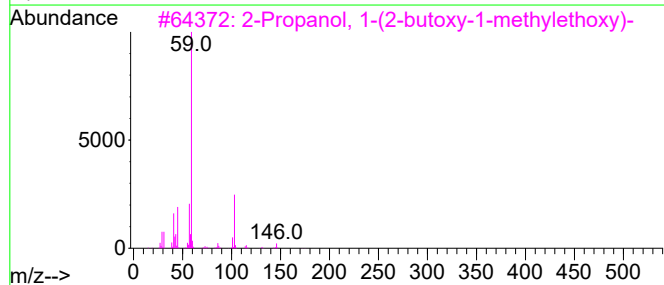
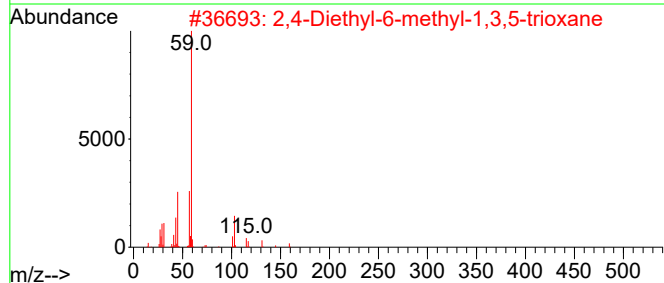
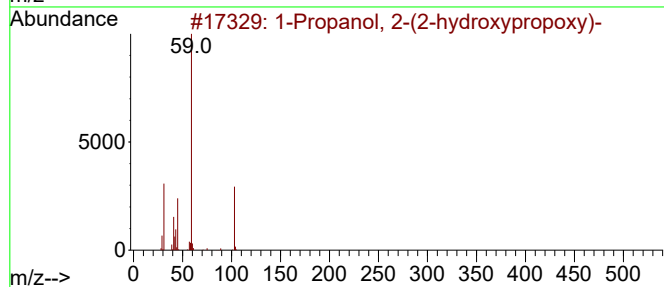
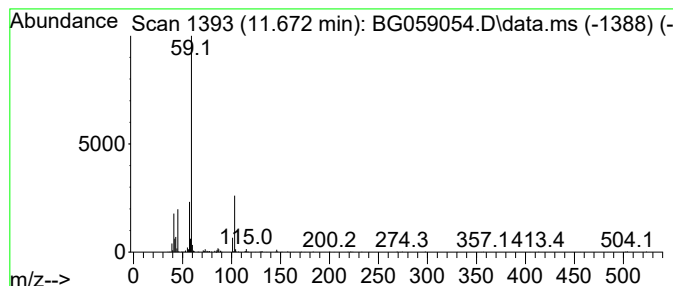
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol, 2-(2-hydroxypro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.672	16.23 ng/ul	750070	Naphthalene-d8	11.143

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78		
2	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	78		
3	2-Propanol, 1-(2-butoxy-1-methyl...)	190	C10H22O3	029911-28-2	78		
4	2-Propanol, 1,1'-[(1-methyl-1,2-...]	192	C9H20O4	001638-16-0	72		
5	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	64		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091323\
Data File : BG059054.D
Acq On : 14 Sep 2023 00:54
Operator : MA/JU
Sample : 04280-01 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JLAD0

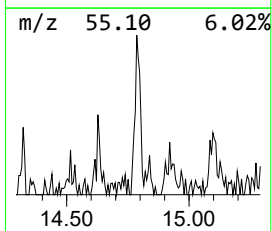
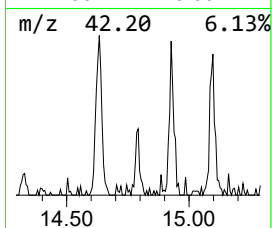
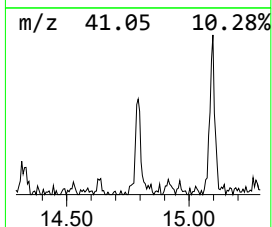
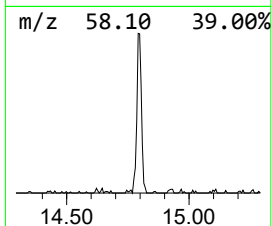
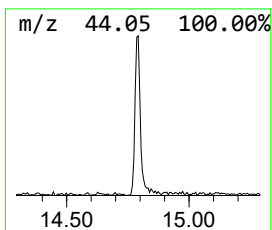
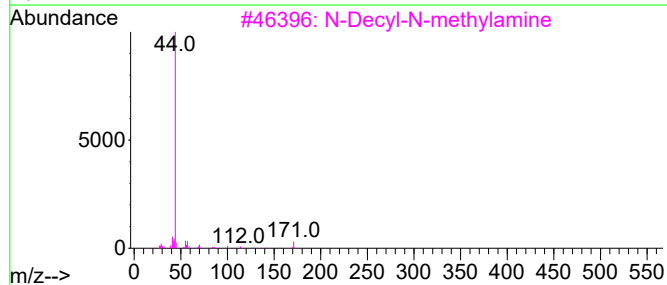
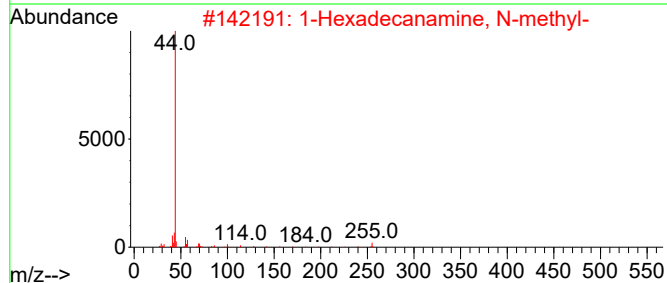
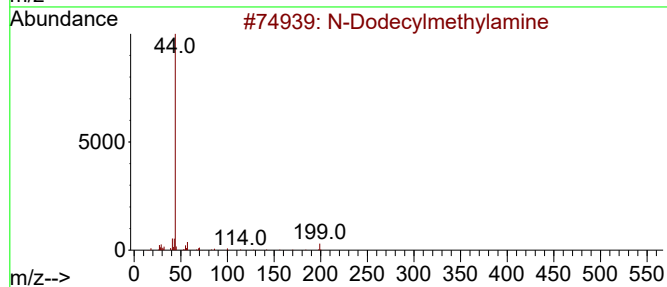
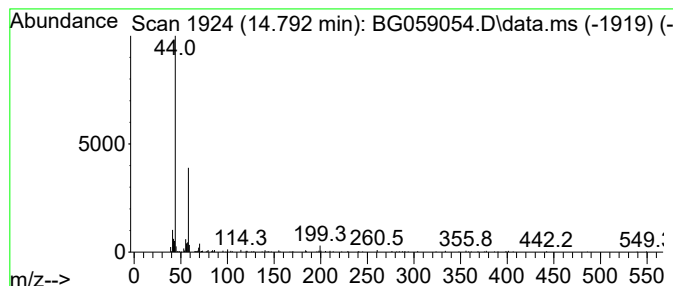
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091023.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	2.53 ng/ul	188421	Acenaphthene-d10	14.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Dodecylmethylamine	199	C13H29N	1000342-26-1	46
2			1-Hexadecanamine, N-methyl-	255	C17H37N	013417-08-8	43
3			N-Decyl-N-methylamine	171	C11H25N	007516-82-7	43
4			1-Methyldodecylamine	199	C13H29N	013205-57-7	43
5			1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091323\
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Sample : 04280-01 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JLAD0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091023.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetylacetone	3.963	2.5	ng/ul	70849	1	8.305	576522	20.0
Propanoic acid,...	5.279	3.3	ng/ul	95874	1	8.305	576522	20.0
2-Propanol, 1-...	11.613	13.6	ng/ul	626344	2	11.143	924380	20.0
1-Propanol, 2-...	11.672	16.2	ng/ul	750070	2	11.143	924380	20.0
unknown-01	14.792	2.5	ng/ul	188421	3	14.927	1487290	20.0