

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100523\
 Data File : BG059322.D
 Acq On : 6 Oct 2023 9:12
 Operator : MA/JU
 Sample : 04592-03 10X
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EZYY1

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-BG092723.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG059322.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.543	22	26	27	rBV4	7533	8449	0.48%	0.046%
2	3.889	82	85	90	rVB2	9628	14879	0.84%	0.082%
3	3.971	93	99	113	rBV2	75033	161421	9.10%	0.884%
4	4.165	129	132	133	rBV2	4600	4231	0.24%	0.023%
5	4.265	146	149	150	rBV3	5065	5979	0.34%	0.033%
6	4.400	169	172	174	rBV4	3222	4146	0.23%	0.023%
7	4.447	179	180	186	rVB6	5183	7023	0.40%	0.038%
8	4.565	193	200	207	rVB3	18764	39752	2.24%	0.218%
9	4.812	239	242	243	rBV	4605	4681	0.26%	0.026%
10	4.847	243	248	255	rVB6	9449	18673	1.05%	0.102%
11	5.158	298	301	302	rBV2	4217	3491	0.20%	0.019%
12	5.211	305	310	317	rVB3	18311	34216	1.93%	0.187%
13	5.264	317	319	320	rBV	4981	4006	0.23%	0.022%
14	5.693	390	392	395	rBV3	2875	3403	0.19%	0.019%
15	5.846	414	418	425	rVB5	3729	8007	0.45%	0.044%
16	6.492	524	528	530	rBV2	2471	3808	0.21%	0.021%
17	6.633	548	552	555	rBV3	2476	4081	0.23%	0.022%
18	6.751	569	572	577	rVB4	2371	3474	0.20%	0.019%
19	6.903	595	598	603	rBV3	3673	5783	0.33%	0.032%
20	7.362	670	676	688	rVB2	68719	130064	7.33%	0.713%
21	7.555	703	709	716	rBV	231870	388508	21.91%	2.129%
22	7.749	735	742	753	rBV	221123	398697	22.48%	2.184%
23	8.120	799	805	807	rVB2	2153	4130	0.23%	0.023%
24	8.231	818	824	833	rVV	217725	383169	21.61%	2.099%
25	8.924	934	942	951	rBV2	184459	325457	18.35%	1.783%
26	9.077	964	968	976	rVV4	9192	14892	0.84%	0.082%
27	9.259	996	999	1002	rBV2	3134	3896	0.22%	0.021%
28	9.430	1020	1028	1041	rBV	298502	541461	30.53%	2.967%
29	9.582	1052	1054	1058	rVV3	4264	5614	0.32%	0.031%
30	9.641	1060	1064	1074	rVB3	7643	14589	0.82%	0.080%
31	9.853	1097	1100	1102	rBV2	4478	5348	0.30%	0.029%
32	10.147	1140	1150	1158	rBV2	223075	411695	23.22%	2.256%
33	10.317	1176	1179	1180	rBV2	3800	4680	0.26%	0.026%
34	10.440	1199	1200	1203	rBV2	3034	3532	0.20%	0.019%
35	10.622	1228	1231	1232	rBV	9170	7086	0.40%	0.039%
36	10.675	1234	1240	1248	rVB	315026	568489	32.06%	3.115%

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37	10.946	1277	1286	1289	rBV4	7270	14861	0.84%	0.081%
38	11.075	1301	1308	1315	rVV	304768	546731	30.83%	2.995%
39	11.216	1323	1332	1341	rBV	302392	557314	31.43%	3.053%
40	11.433	1366	1369	1371	rBV	2898	3374	0.19%	0.018%
41	11.539	1379	1387	1392	rBV2	33322	58189	3.28%	0.319%
42	11.598	1392	1397	1406	rVB3	40122	69943	3.94%	0.383%
43	11.792	1426	1430	1432	rBV2	4654	6431	0.36%	0.035%
44	11.815	1432	1434	1438	rVB3	4171	5566	0.31%	0.030%
45	11.856	1438	1441	1442	rBV2	3129	3538	0.20%	0.019%
46	12.367	1524	1528	1533	rBV3	12511	19471	1.10%	0.107%
47	12.432	1537	1539	1543	rVB2	2453	3464	0.20%	0.019%
48	12.638	1569	1574	1578	rVB2	9729	14883	0.84%	0.082%
49	12.720	1583	1588	1591	rBV4	4733	6882	0.39%	0.038%
50	13.178	1662	1666	1668	rBV2	2730	3548	0.20%	0.019%
51	13.613	1736	1740	1741	rBV3	5543	5009	0.28%	0.027%
52	13.654	1744	1747	1749	rVV3	6263	7684	0.43%	0.042%
53	13.695	1749	1754	1759	rVB3	23717	38840	2.19%	0.213%
54	14.036	1809	1812	1816	rVB5	4583	7000	0.39%	0.038%
55	14.177	1832	1836	1837	rBV4	4360	6260	0.35%	0.034%
56	14.259	1843	1850	1855	rBV	598163	869906	49.05%	4.766%
57	14.306	1856	1858	1864	rVB2	14097	16402	0.92%	0.090%
58	14.494	1887	1890	1894	rBV3	2443	3951	0.22%	0.022%
59	14.571	1894	1903	1909	rBV2	725365	1165304	65.71%	6.385%
60	14.865	1947	1953	1960	rVV	464372	702286	39.60%	3.848%
61	15.058	1980	1986	1991	rBV2	49158	84093	4.74%	0.461%
62	15.217	2007	2013	2015	rBV3	7522	11772	0.66%	0.064%
63	15.458	2051	2054	2059	rVB2	4254	5874	0.33%	0.032%
64	15.505	2059	2062	2064	rBV2	2866	3376	0.19%	0.018%
65	15.622	2080	2082	2087	rVB4	9209	12879	0.73%	0.071%
66	15.693	2091	2094	2095	rVV2	4477	4363	0.25%	0.024%
67	15.734	2099	2101	2104	rVB2	4196	3801	0.21%	0.021%
68	15.852	2114	2121	2128	rBV	946862	1398894	78.88%	7.664%
69	15.963	2135	2140	2151	rBV2	232507	350190	19.75%	1.919%
70	16.087	2157	2161	2162	rBV3	6594	6064	0.34%	0.033%
71	16.145	2168	2171	2173	rBV	4076	4232	0.24%	0.023%
72	16.492	2227	2230	2233	rVB4	3493	3458	0.19%	0.019%
73	16.633	2252	2254	2256	rBV3	4034	4309	0.24%	0.024%
74	16.727	2268	2270	2273	rVB3	6271	6629	0.37%	0.036%
75	16.874	2293	2295	2299	rVB4	3894	4680	0.26%	0.026%
76	16.921	2299	2303	2304	rBV3	3552	3489	0.20%	0.019%

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77	17.197	2345	2350	2351	rBV2	4148	6148	0.35%	0.034%
78	17.497	2399	2401	2403	rBV2	4396	4411	0.25%	0.024%
79	17.556	2410	2411	2414	rBV2	5504	4335	0.24%	0.024%
80	17.614	2414	2421	2428	rVV	558896	840570	47.40%	4.605%
81	17.714	2431	2438	2445	rBV2	1073703	1572258	88.66%	8.614%
82	17.873	2462	2465	2468	rBV4	4807	5673	0.32%	0.031%
83	17.996	2481	2486	2487	rBV4	4228	5466	0.31%	0.030%
84	18.090	2499	2502	2506	rBV4	3345	3978	0.22%	0.022%
85	18.313	2535	2540	2543	rBV7	7943	11272	0.64%	0.062%
86	18.431	2556	2560	2570	rBV	135926	206847	11.66%	1.133%
87	18.595	2586	2588	2590	rBV3	6200	6582	0.37%	0.036%
88	18.701	2604	2606	2610	rBV5	7942	8468	0.48%	0.046%
89	18.866	2632	2634	2636	rBV3	6865	4299	0.24%	0.024%
90	18.966	2649	2651	2653	rBV3	5307	5457	0.31%	0.030%
91	19.594	2755	2758	2762	rBV2	66735	76956	4.34%	0.422%
92	19.694	2771	2775	2779	rBV5	55346	73266	4.13%	0.401%
93	19.835	2795	2799	2803	rBV	220024	241407	13.61%	1.323%
94	19.947	2816	2818	2820	rBV3	23834	23471	1.32%	0.129%
95	19.988	2820	2825	2831	rVB	1284383	1773400	100.00%	9.716%
96	20.664	2937	2940	2943	rVB	44025	48214	2.72%	0.264%
97	20.875	2972	2976	2981	rBV	156983	193139	10.89%	1.058%
98	21.915	3148	3153	3159	rVB2	489666	844120	47.60%	4.625%
99	25.158	3696	3705	3715	rVB	600217	1728771	97.48%	9.472%
100	25.405	3738	3747	3758	rVB4	309251	967795	54.57%	5.302%

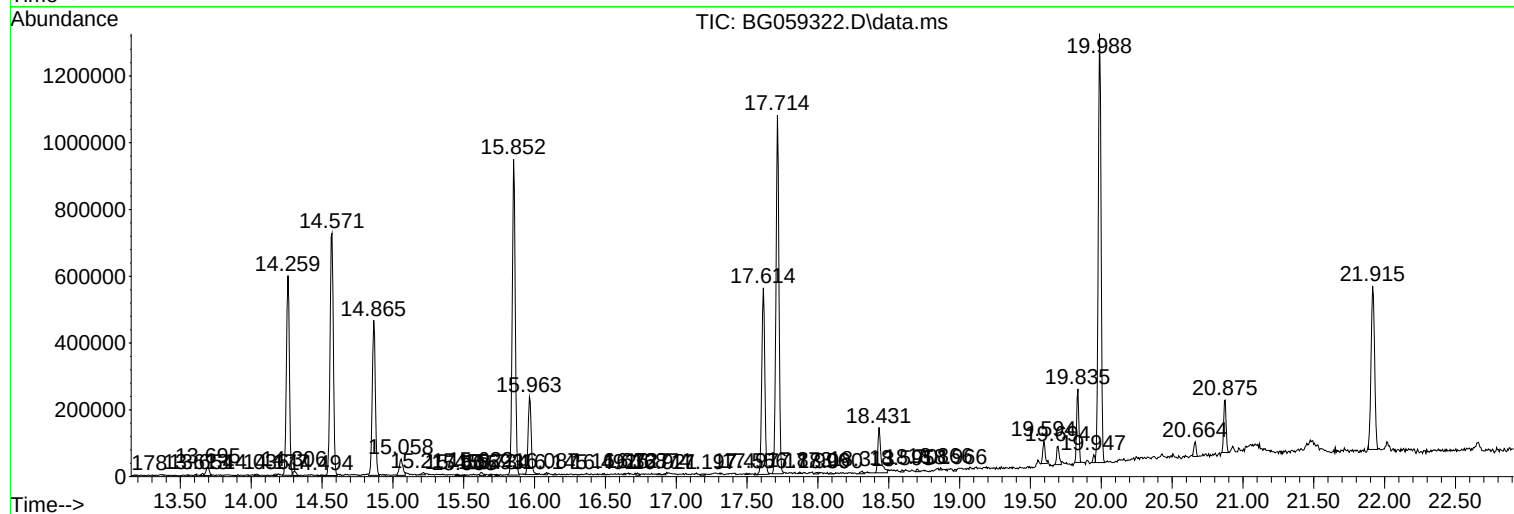
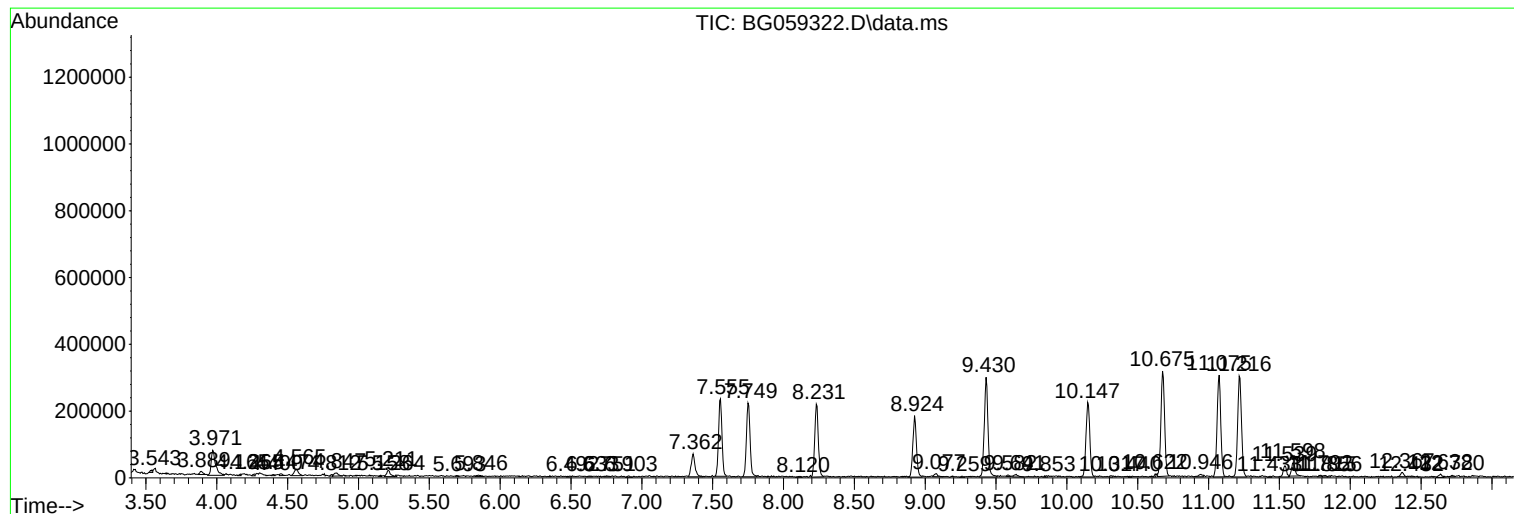
Sum of corrected areas: 18252053

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG092723.MA.M
Quant Title : SVOA CALIBRATION

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



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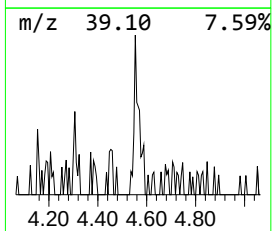
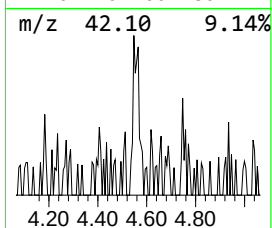
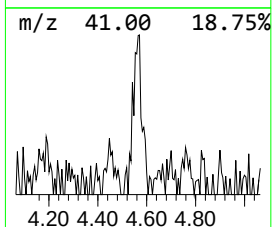
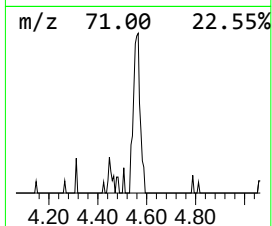
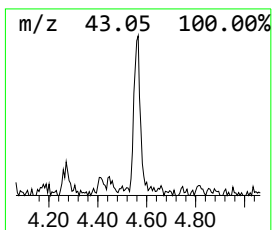
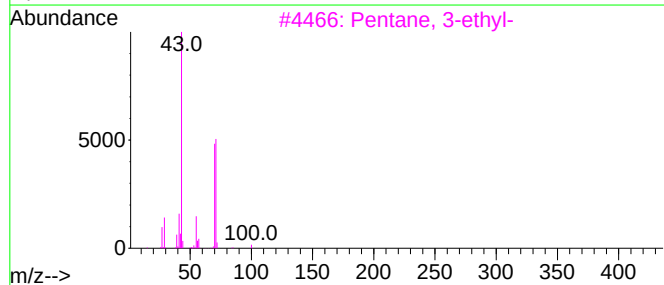
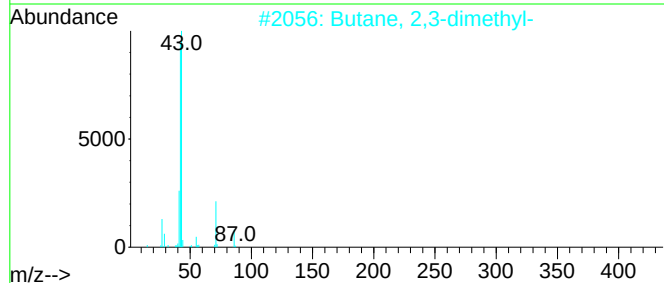
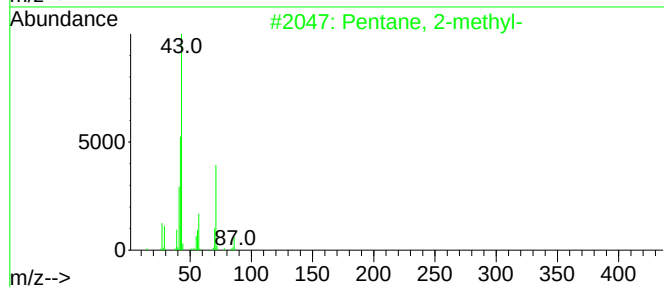
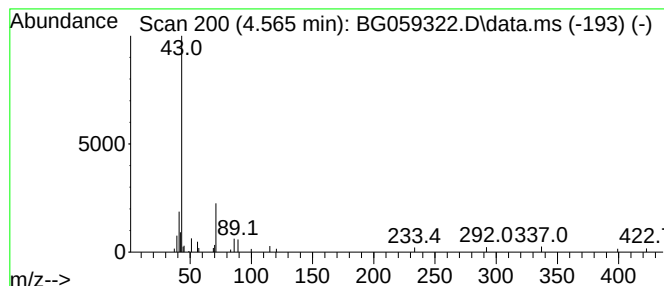
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG092723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.565	2.07 ng/ul	39752	1,4-Dichlorobenzene-d4	8.237

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	9
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	9
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	9
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9



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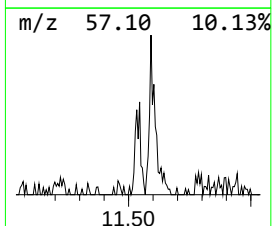
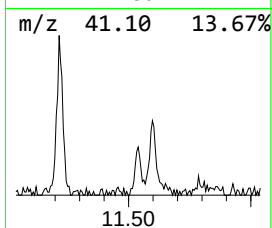
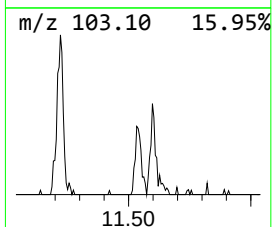
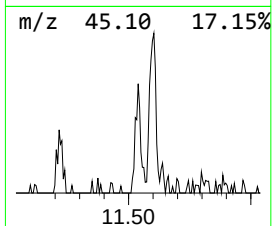
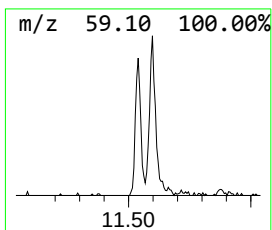
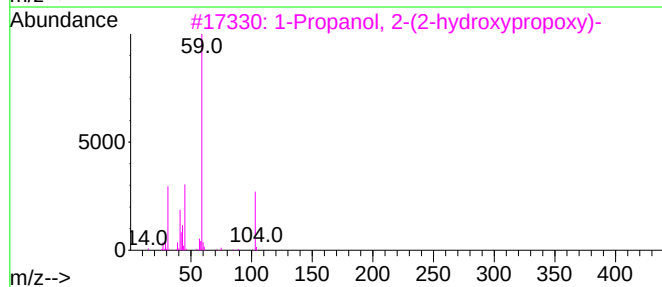
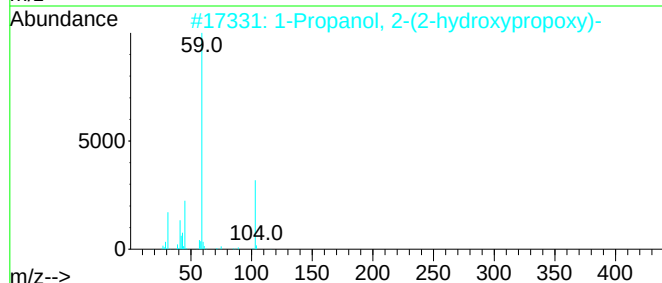
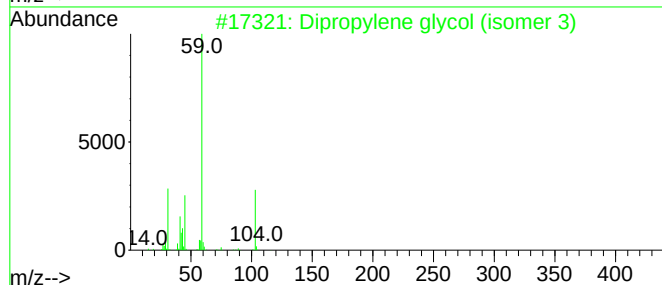
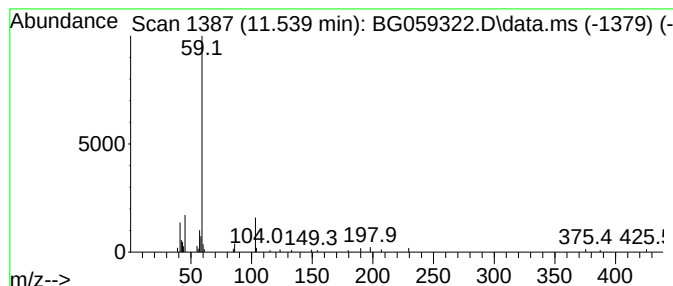
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG092723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Dipropylene glycol (isomer 3) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.539	2.13 ng/ul	58189	Naphthalene-d8	11.075

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	72
2			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
4			1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	72
5			Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	72



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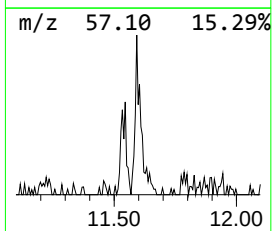
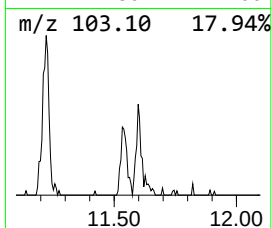
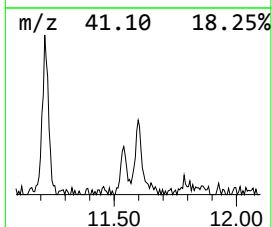
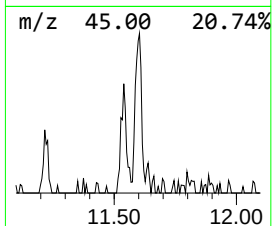
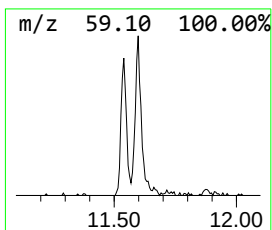
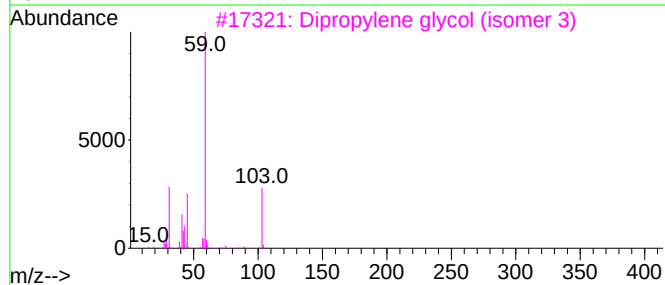
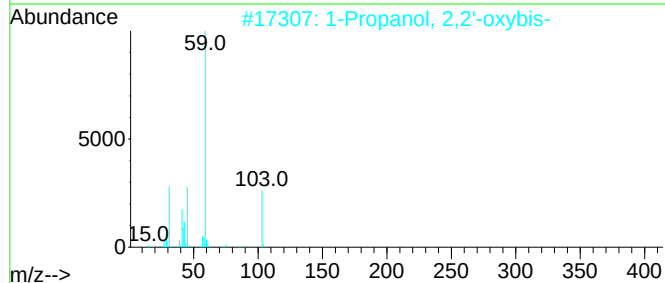
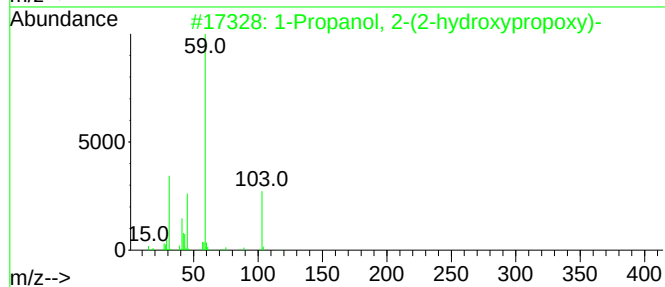
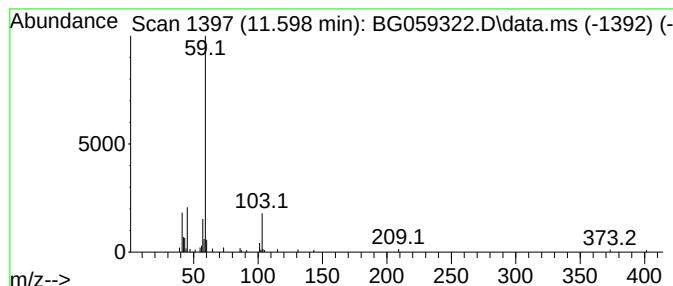
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG092723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 1-Propanol, 2-(2-hydroxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.598	2.56 ng/ul	69943	Naphthalene-d8	11.075

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
2		1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	72
3		Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	72
4		2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	64
5		2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100523\
Data File : BG059322.D
Acq On : 6 Oct 2023 9:12
Operator : MA/JU
Sample : 04592-03 10X
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EZZY1

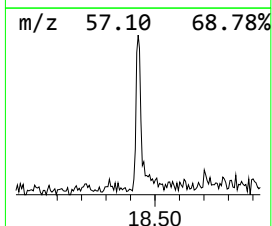
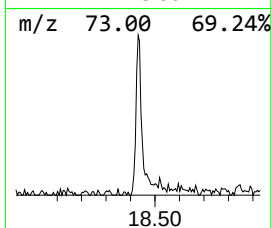
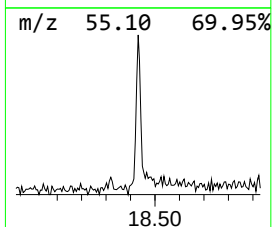
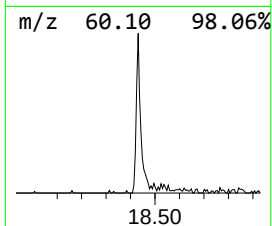
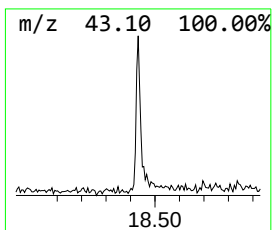
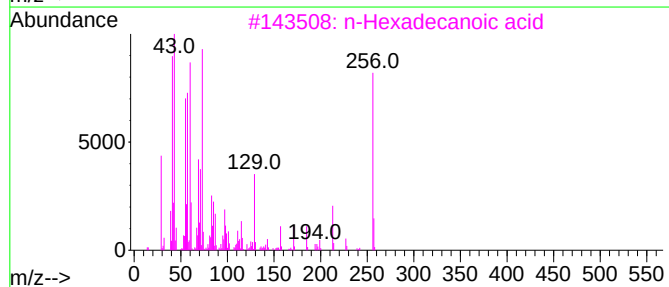
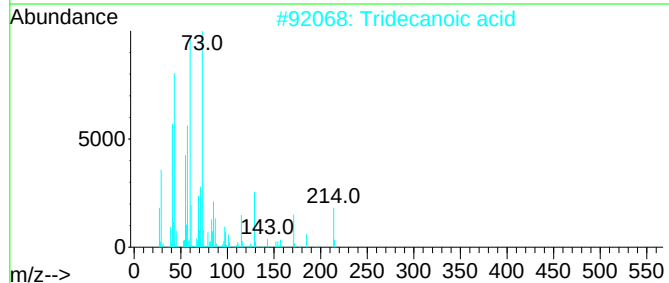
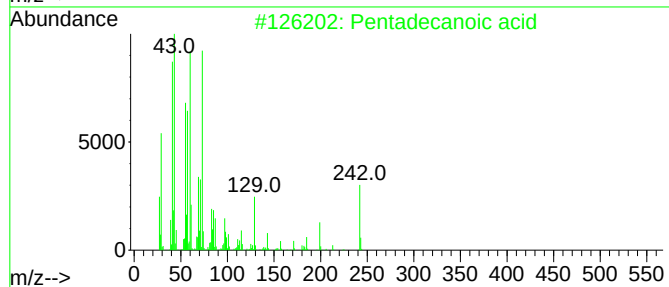
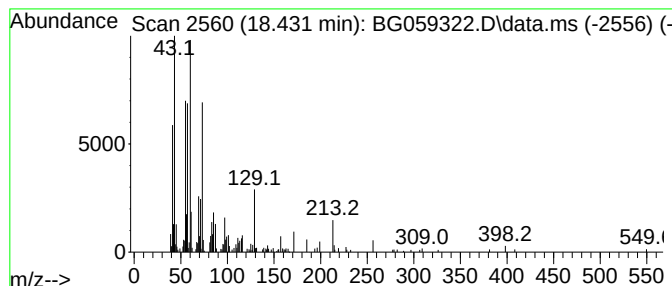
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Pentadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.431	4.92 ng/ul	206847	Phenanthrene-d10	17.614

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
2			Tridecanoic acid	214	C13H26O2	000638-53-9	64
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
4			Octanoic acid	144	C8H16O2	000124-07-2	52
5			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100523\
Data File : BG059322.D
Acq On : 6 Oct 2023 9:12
Operator : MA/JU
Sample : 04592-03 10X
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EZY1

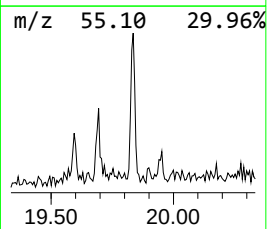
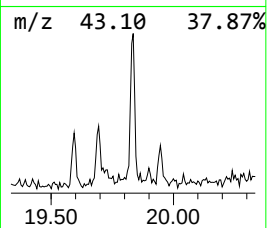
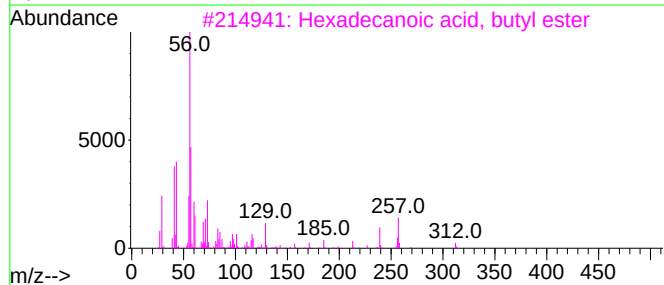
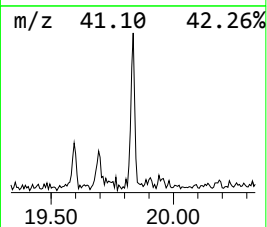
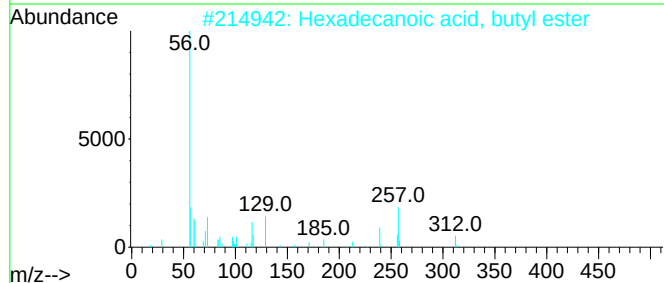
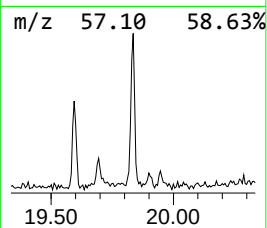
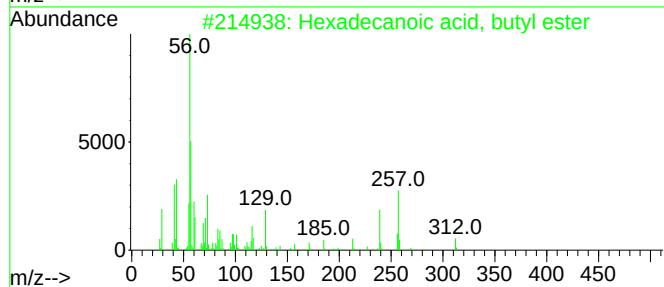
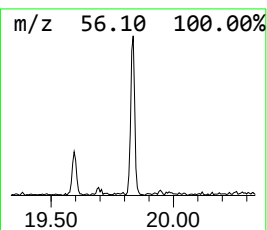
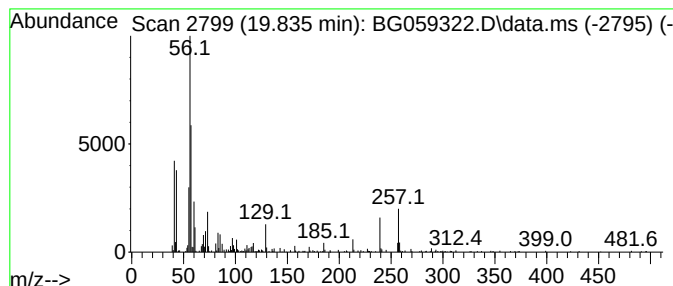
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.835	5.72 ng/ul	241407	Chrysene-d12	21.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	78
3			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	72
4			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	45
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100523\
Data File : BG059322.D
Acq On : 6 Oct 2023 9:12
Operator : MA/JU
Sample : 04592-03 10X
Misc :
ALS Vial : 36 Sample Multiplier: 1

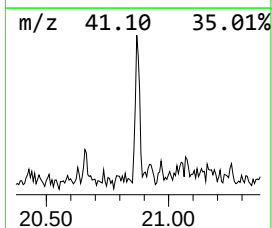
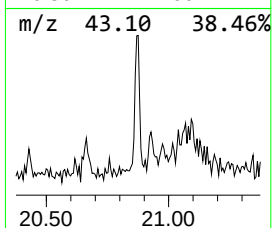
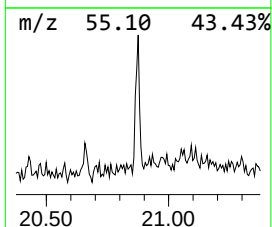
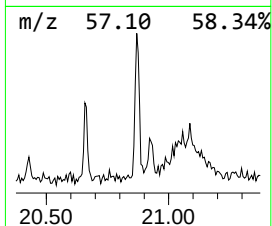
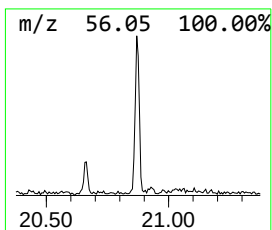
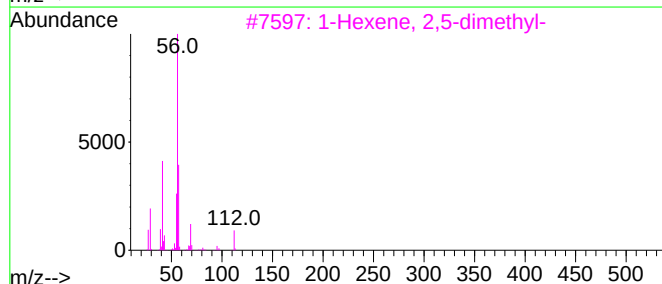
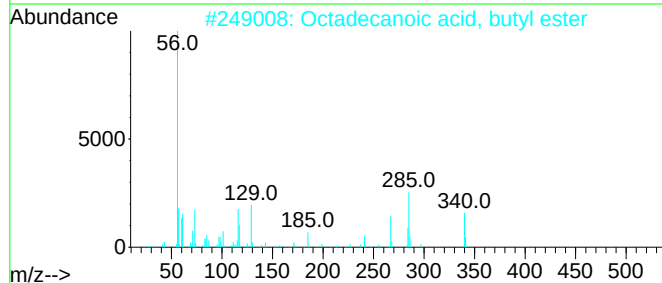
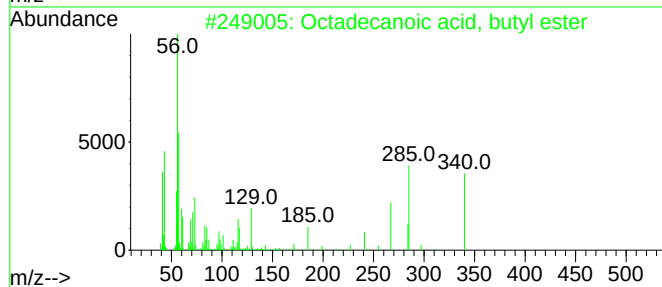
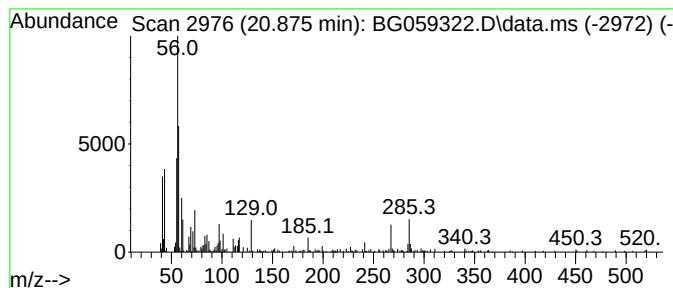
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG092723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.875	4.58 ng/ul	193139	Chrysene-d12	21.915	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	70
2	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	59
3	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	46
4	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	46
5	Tetracosanoic acid, isobutyl ester	424	C28H56O2	1010405-17-3	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100523\
Data File : BG059322.D
Acq On : 6 Oct 2023 9:12
Operator : MA/JU
Sample : 04592-03 10X
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EZY1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG092723.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	4.565	2.1	ng/ul	39752	1	8.237	383169	20.0
Dipropylene gly...	11.539	2.1	ng/ul	58189	2	11.075	546731	20.0
1-Propanol, 2-(...	11.598	2.6	ng/ul	69943	2	11.075	546731	20.0
Pentadecanoic acid	18.431	4.9	ng/ul	206847	4	17.614	840570	20.0
Hexadecanoic ac...	19.835	5.7	ng/ul	241407	5	21.915	844120	20.0
Octadecanoic ac...	20.875	4.6	ng/ul	193139	5	21.915	844120	20.0