

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
 Data File : BG062288.D
 Acq On : 7 Aug 2024 3:53
 Operator : MA/JU
 Sample : P3336-07
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 F7E32

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-BG080524.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG062288.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.423	19	23	29	rVB2	14714	21878	0.88%	0.090%
2	3.682	63	67	77	rBV	78688	125590	5.04%	0.517%
3	3.829	87	92	103	rBV	203359	339726	13.63%	1.398%
4	4.169	148	150	154	rVB2	3895	3913	0.16%	0.016%
5	5.074	299	304	308	rVB3	2960	4248	0.17%	0.017%
6	6.043	464	469	476	rVB2	8448	13248	0.53%	0.055%
7	7.112	644	651	662	rBV	333674	569693	22.86%	2.345%
8	7.289	674	681	691	rVB	232564	381695	15.32%	1.571%
9	7.488	708	715	723	rBV	298658	509566	20.45%	2.097%
10	7.553	723	726	731	rVV	13106	21853	0.88%	0.090%
11	7.958	786	795	802	rBV	175451	300236	12.05%	1.236%
12	8.017	802	805	811	rVB4	7375	11703	0.47%	0.048%
13	8.652	906	913	927	rBV	404042	701157	28.14%	2.886%
14	9.110	984	991	999	rBV	300996	525547	21.09%	2.163%
15	9.286	1016	1021	1024	rBV4	1931	2895	0.12%	0.012%
16	9.568	1066	1069	1074	rVB3	2882	4225	0.17%	0.017%
17	9.674	1081	1087	1096	rBV	34350	54206	2.18%	0.223%
18	9.832	1106	1114	1128	rBV	241557	427290	17.15%	1.759%
19	10.367	1197	1205	1217	rBV	418094	742279	29.79%	3.055%
20	10.525	1228	1232	1238	rVB2	2334	3457	0.14%	0.014%
21	10.755	1263	1271	1280	rBV	281829	501956	20.14%	2.066%
22	10.878	1283	1292	1302	rBV	426394	768988	30.86%	3.165%
23	11.289	1357	1362	1367	rBV2	12869	19882	0.80%	0.082%
24	11.489	1389	1396	1404	rBV2	77873	135018	5.42%	0.556%
25	12.335	1535	1540	1547	rVB3	7588	10872	0.44%	0.045%
26	13.427	1721	1726	1730	rBV4	4652	8069	0.32%	0.033%
27	13.551	1744	1747	1751	rBV	1637	2611	0.10%	0.011%
28	13.986	1815	1821	1829	rBV	782610	1171604	47.02%	4.823%
29	14.273	1856	1870	1877	rBV	950237	1496204	60.04%	6.159%
30	14.491	1904	1907	1913	rBV3	2791	3607	0.14%	0.015%
31	14.579	1915	1922	1929	rVV	510547	788476	31.64%	3.246%
32	14.755	1944	1952	1956	rBV	361825	579887	23.27%	2.387%
33	14.808	1956	1961	1966	rVB2	55904	120542	4.84%	0.496%
34	14.990	1987	1992	1999	rVB7	8057	13557	0.54%	0.056%
35	15.384	2055	2059	2066	rBV3	4759	8093	0.32%	0.033%
36	15.442	2066	2069	2073	rBV4	2632	4016	0.16%	0.017%

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37	15.572	2084	2091	2098	rBV	1220969	1878868	75.40%	7.734%
38	15.624	2098	2100	2103	rVV2	3836	4122	0.17%	0.017%
39	15.677	2103	2109	2119	rVB	249321	376106	15.09%	1.548%
40	15.812	2128	2132	2135	rBV4	3941	5073	0.20%	0.021%
41	15.953	2152	2156	2161	rVB5	1589	3108	0.12%	0.013%
42	16.012	2161	2166	2169	rVB3	2729	4650	0.19%	0.019%
43	16.130	2182	2186	2192	rBV4	2947	5130	0.21%	0.021%
44	16.194	2194	2197	2201	rBV2	1603	2595	0.10%	0.011%
45	16.306	2212	2216	2219	rBV2	4818	5490	0.22%	0.023%
46	16.887	2310	2315	2319	rBV3	5344	7906	0.32%	0.033%
47	17.046	2340	2342	2346	rVB5	3152	3205	0.13%	0.013%
48	17.099	2346	2351	2354	rBV3	4601	7126	0.29%	0.029%
49	17.128	2354	2356	2363	rVB2	2749	4327	0.17%	0.018%
50	17.316	2381	2388	2398	rVV	643607	955624	38.35%	3.934%
51	17.416	2398	2405	2416	rVV2	1343019	1988900	79.81%	8.187%
52	17.504	2416	2420	2425	rVB2	8622	12275	0.49%	0.051%
53	17.639	2440	2443	2447	rVB3	3012	3883	0.16%	0.016%
54	17.839	2474	2477	2480	rBV3	1889	2567	0.10%	0.011%
55	18.004	2500	2505	2509	rBV3	7271	9499	0.38%	0.039%
56	18.221	2537	2542	2553	rBV	145424	236037	9.47%	0.972%
57	18.385	2566	2570	2574	rVB3	3415	4704	0.19%	0.019%
58	18.532	2591	2595	2599	rBV5	2924	3543	0.14%	0.015%
59	18.885	2652	2655	2661	rBV7	2044	3460	0.14%	0.014%
60	19.026	2675	2679	2682	rBV5	3969	4452	0.18%	0.018%
61	19.173	2701	2704	2712	rVB7	3493	6089	0.24%	0.025%
62	19.267	2715	2720	2725	rBV2	17726	25593	1.03%	0.105%
63	19.337	2728	2732	2734	rBV	17121	25624	1.03%	0.105%
64	19.366	2734	2737	2742	rVB	16869	23765	0.95%	0.098%
65	19.496	2754	2759	2769	rBV	38078	65187	2.62%	0.268%
66	19.654	2782	2786	2787	rBV4	4462	5027	0.20%	0.021%
67	19.701	2787	2794	2802	rVV	1655026	2396235	96.16%	9.863%
68	19.760	2802	2804	2808	rVB4	6845	7605	0.31%	0.031%
69	20.054	2853	2854	2859	rBV4	1730	2553	0.10%	0.011%
70	20.224	2879	2883	2886	rBV4	8632	11352	0.46%	0.047%
71	20.265	2886	2890	2893	rVB3	5419	7485	0.30%	0.031%
72	20.688	2959	2962	2966	rBV6	5802	7439	0.30%	0.031%
73	20.735	2967	2970	2971	rBV2	4553	4769	0.19%	0.020%
74	20.759	2971	2974	2977	rVB	16806	18453	0.74%	0.076%
75	20.864	2990	2992	2999	rVB7	5451	8174	0.33%	0.034%
76	20.911	2999	3000	3002	rBV2	2660	2544	0.10%	0.010%

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77	21.240	3051	3056	3067	rBV2	217519	344049	13.81%	1.416%
78	21.558	3103	3110	3118	rBV2	674479	1085990	43.58%	4.470%
79	21.722	3136	3138	3139	rBV2	4492	4360	0.17%	0.018%
80	21.793	3144	3150	3156	rBV	42787	66015	2.65%	0.272%
81	22.386	3246	3251	3259	rBV2	48749	92134	3.70%	0.379%
82	23.061	3361	3366	3376	rVB2	36197	69493	2.79%	0.286%
83	23.232	3393	3395	3396	rBV2	5425	4161	0.17%	0.017%
84	23.849	3493	3500	3507	rBV2	38963	82620	3.32%	0.340%
85	24.442	3590	3601	3618	rBV	921438	2491902	100.00%	10.257%
86	24.653	3626	3637	3649	rVV	433622	1155461	46.37%	4.756%
87	24.765	3650	3656	3665	rVV3	29893	77219	3.10%	0.318%
88	24.841	3667	3669	3672	rVB4	4593	2781	0.11%	0.011%
89	25.869	3836	3844	3851	rBV4	26829	72765	2.92%	0.300%
90	25.975	3854	3862	3869	rBV4	17464	52626	2.11%	0.217%
91	27.179	4061	4067	4079	rVB5	19625	61653	2.47%	0.254%
92	28.777	4324	4339	4347	rBV8	18414	72357	2.90%	0.298%
93	28.918	4361	4363	4365	rBV3	3501	3451	0.14%	0.014%
94	32.155	4912	4914	4917	rBV4	2648	3267	0.13%	0.013%
95	32.325	4942	4943	4949	rVB6	2834	3339	0.13%	0.014%

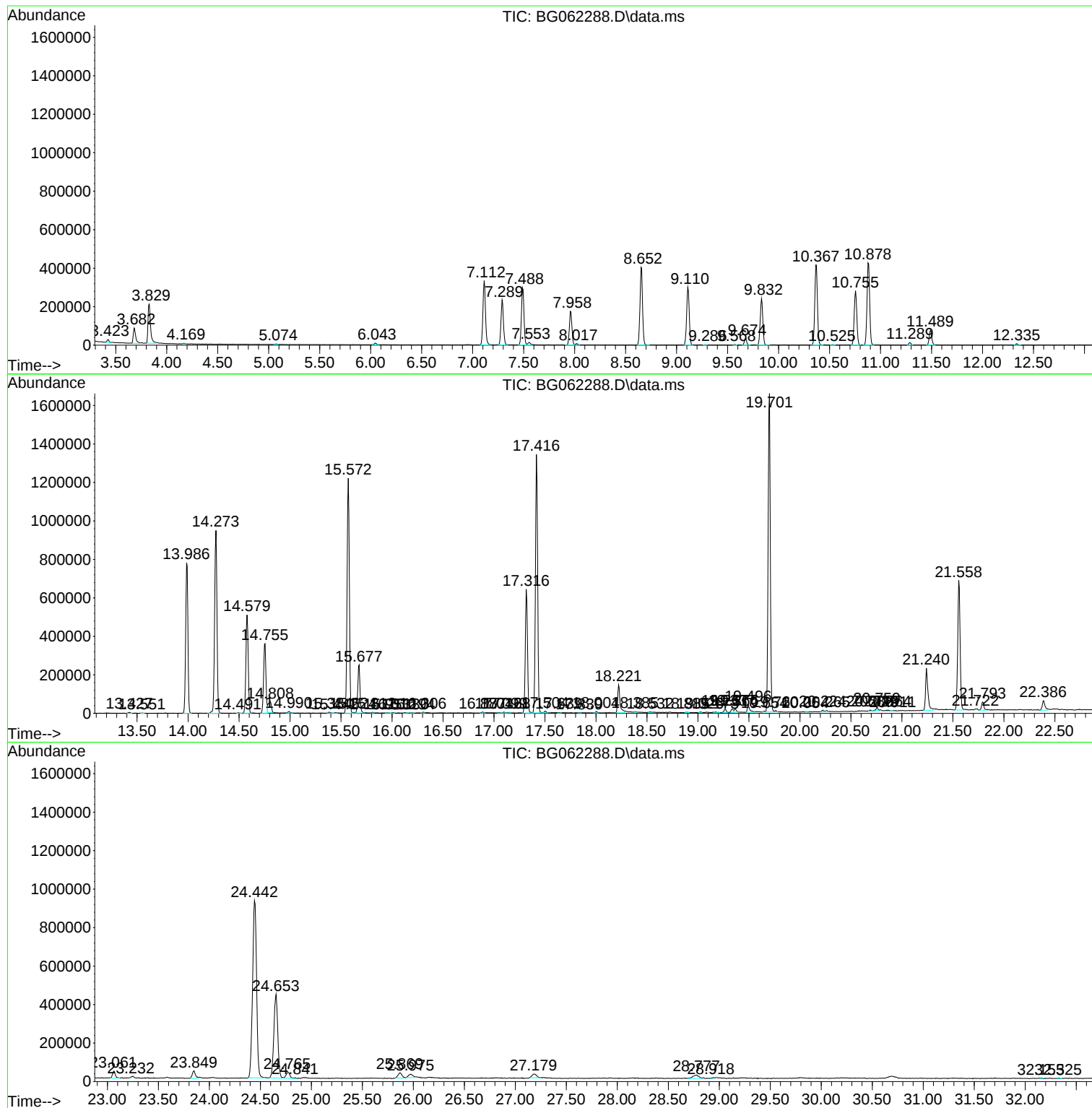
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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



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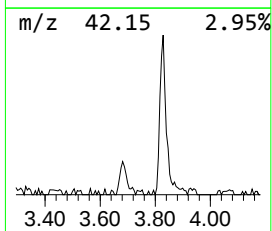
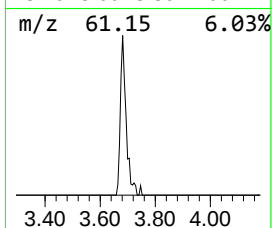
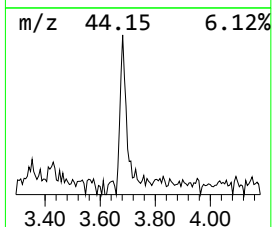
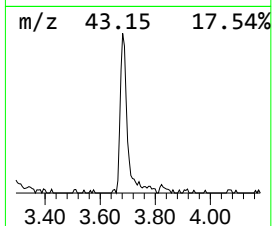
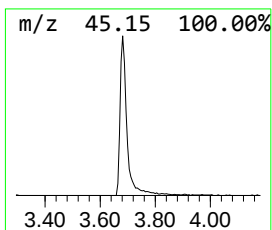
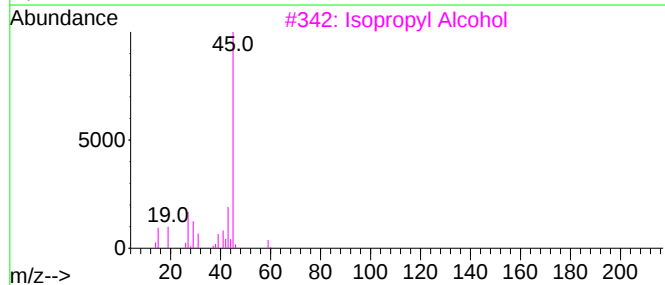
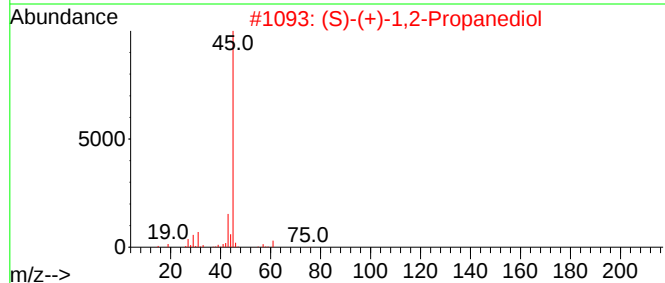
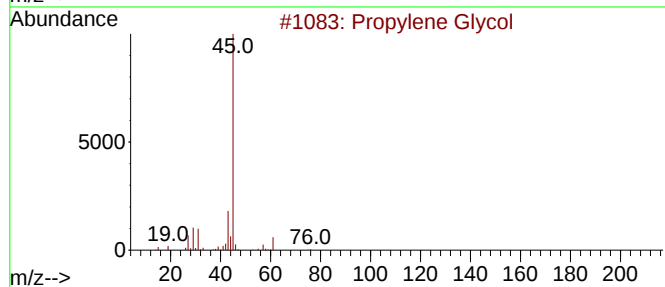
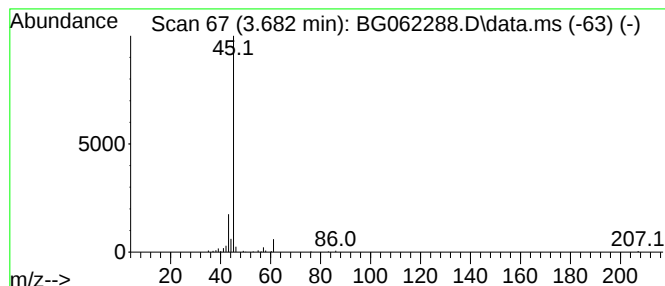
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.682	8.37 ng/ul	125590	1,4-Dichlorobenzene-d4	7.958

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	80
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	50
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
5			Isopropyl Alcohol	60	C3H8O	000067-63-0	9



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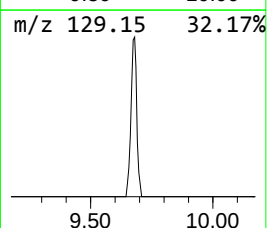
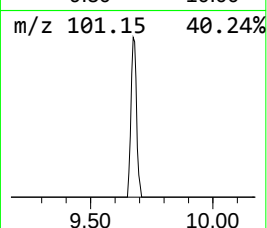
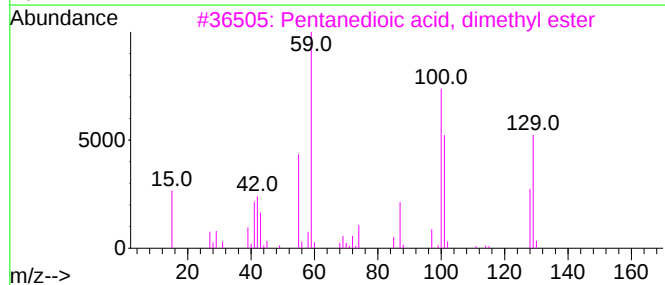
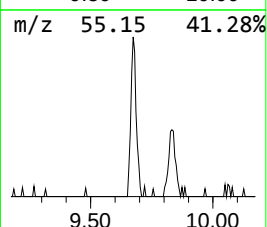
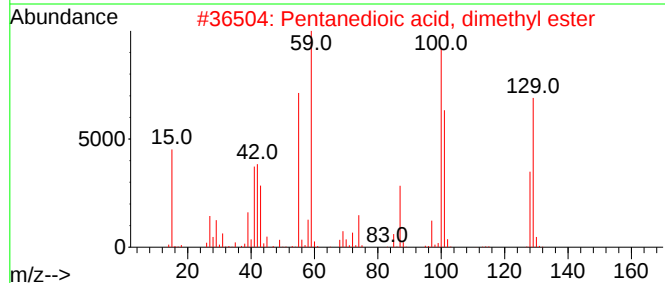
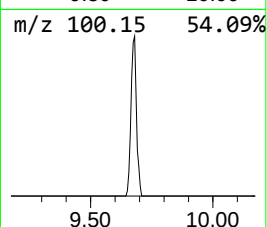
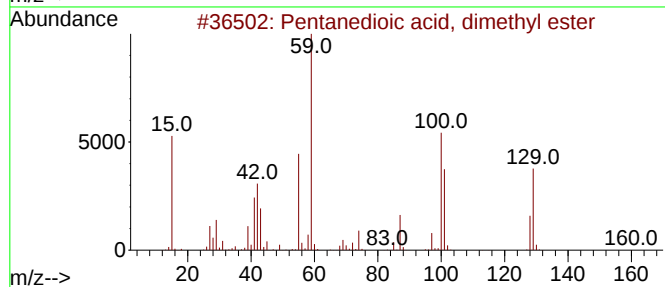
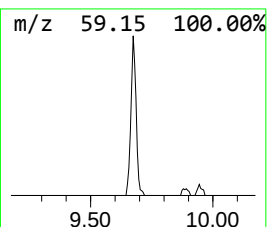
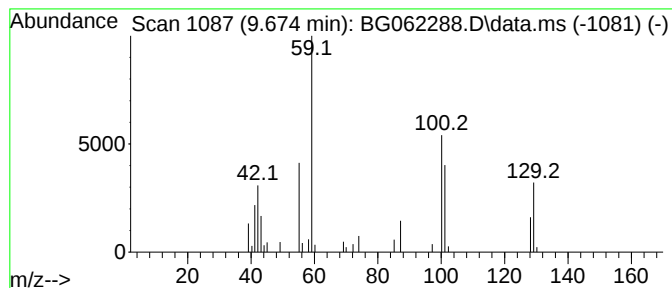
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Pentanedioic acid, dimethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.674	2.16 ng/ul	54206	Naphthalene-d8	10.755

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	90
2			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	45
3			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	40
4			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	40
5			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	40



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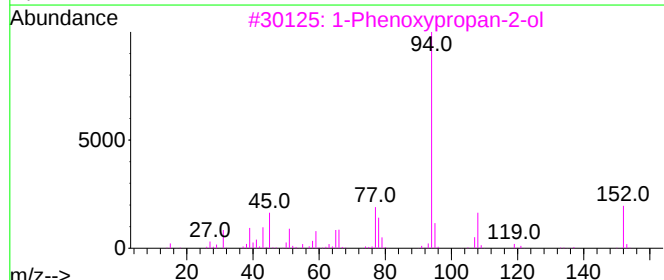
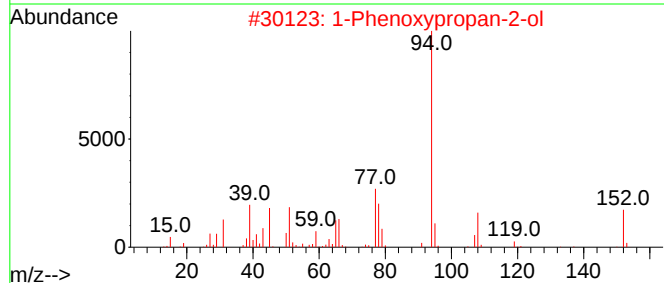
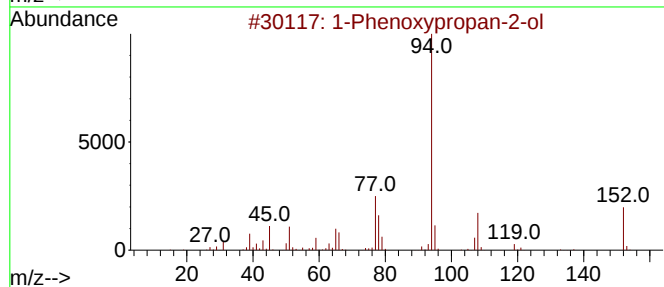
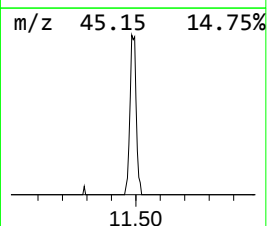
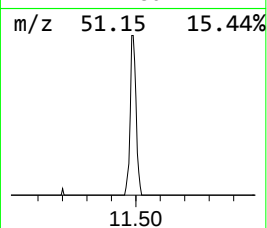
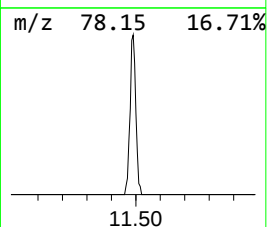
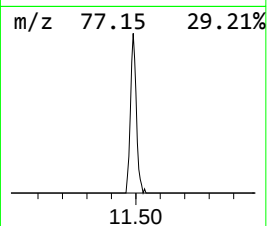
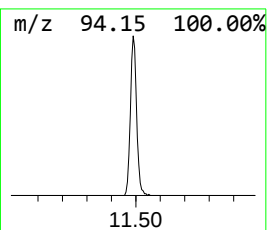
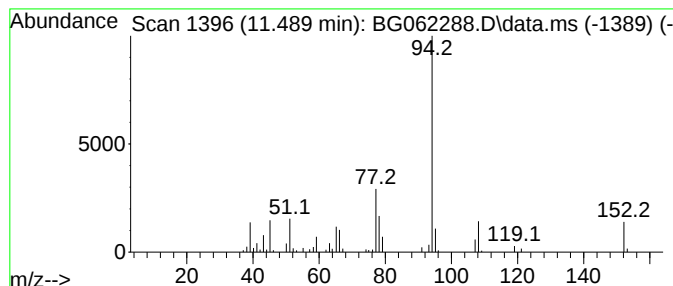
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.489	5.38 ng/ul	135018	Naphthalene-d8	10.755

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
3			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
4			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	72
5			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
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Acq On : 7 Aug 2024 3:53
Operator : MA/JU
Sample : P3336-07
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E32

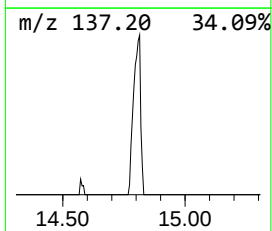
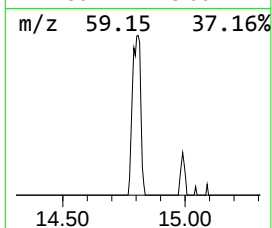
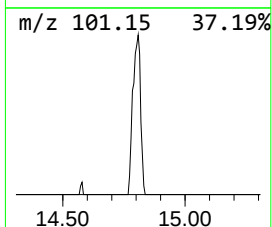
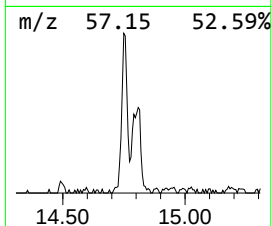
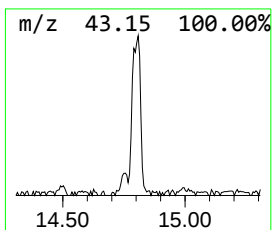
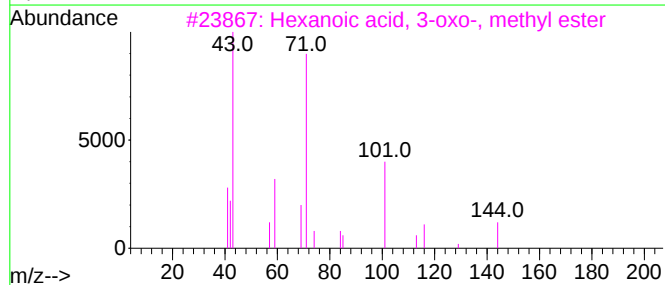
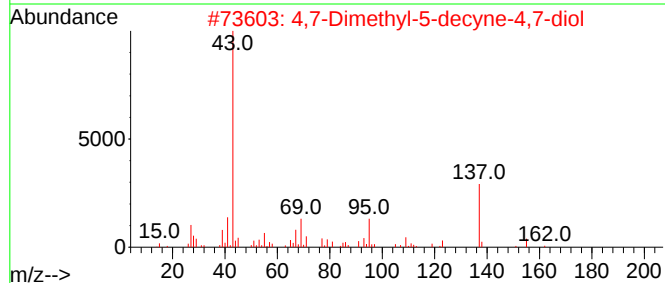
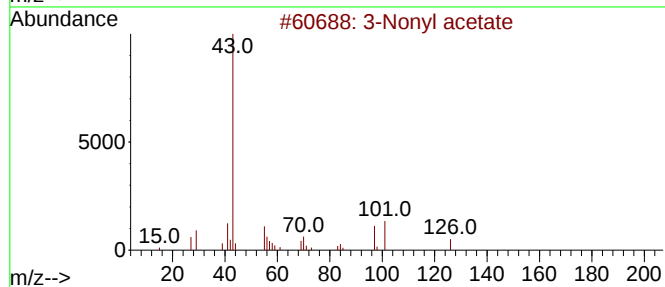
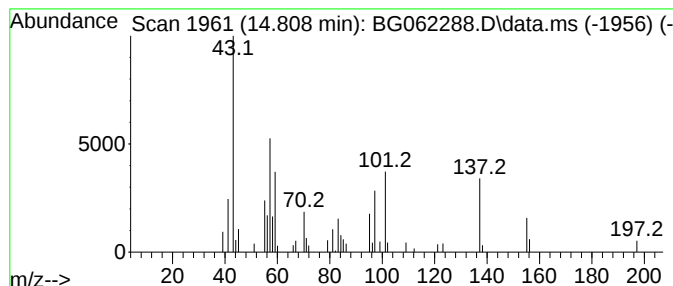
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.808	3.06 ng/ul	120542	Acenaphthene-d10	14.579

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Nonyl acetate	186	C11H22O2	1010429-16-2	22
2			4,7-Dimethyl-5-decyne-4,7-diol	198	C12H22O2	000126-87-4	22
3			Hexanoic acid, 3-oxo-, methyl ester	144	C7H12O3	030414-54-1	10
4			Acetic acid, 3-hydroxy-2-nitroph...	197	C8H7NO5	1000269-41-1	10
5			3-Octanol, acetate	172	C10H20O2	004864-61-3	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
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Acq On : 7 Aug 2024 3:53
Operator : MA/JU
Sample : P3336-07
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E32

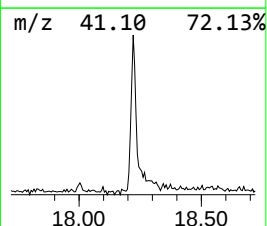
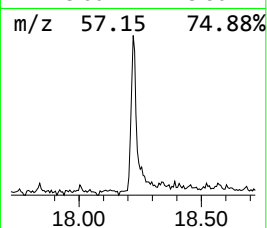
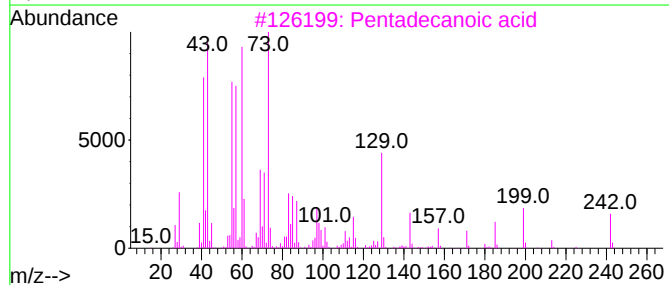
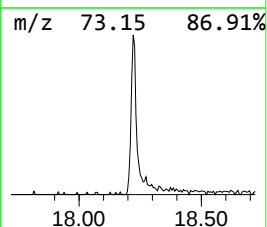
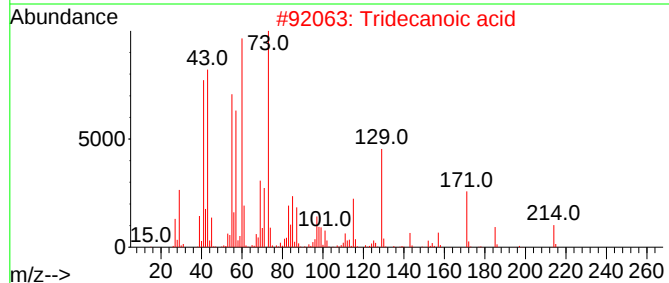
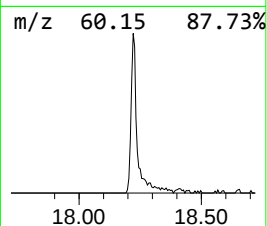
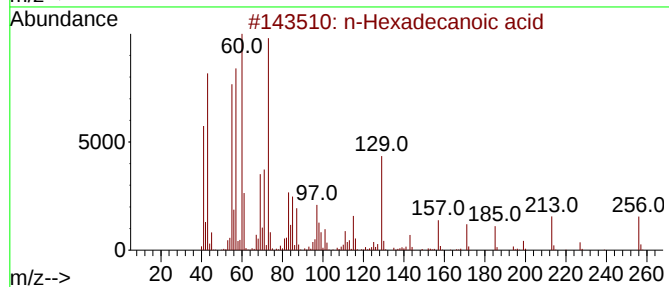
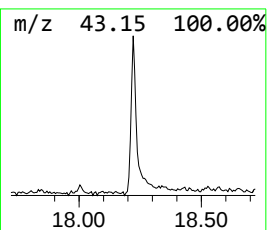
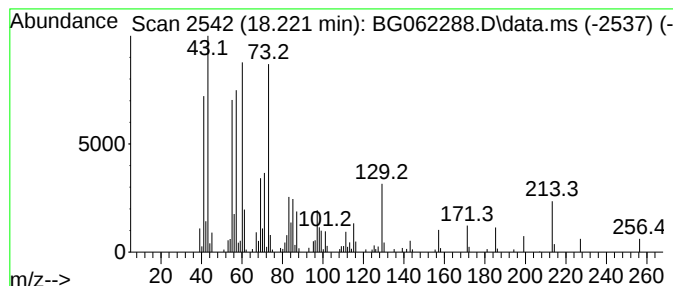
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.221	4.94 ng/ul	236037	Phenanthrene-d10	17.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062288.D
Acq On : 7 Aug 2024 3:53
Operator : MA/JU
Sample : P3336-07
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E32

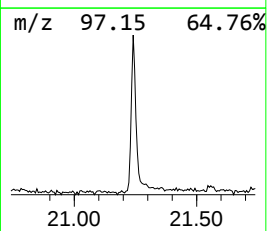
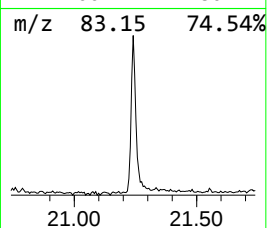
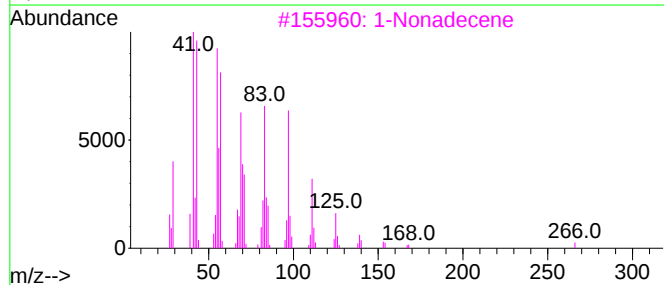
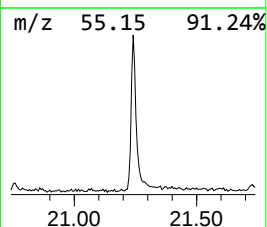
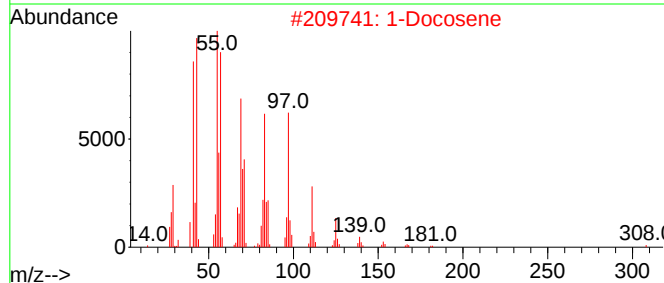
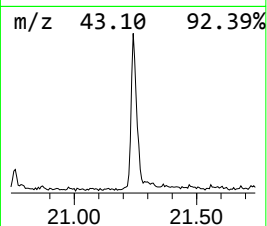
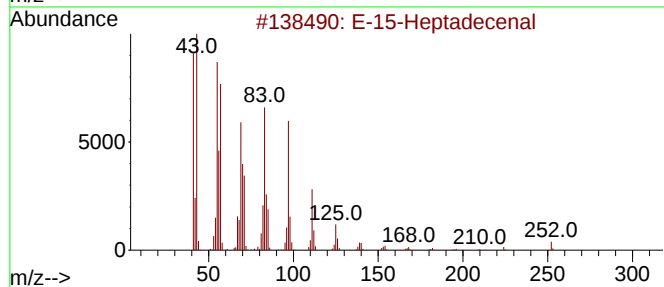
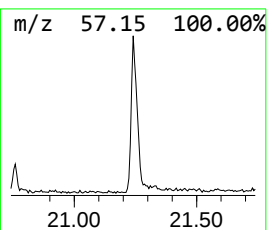
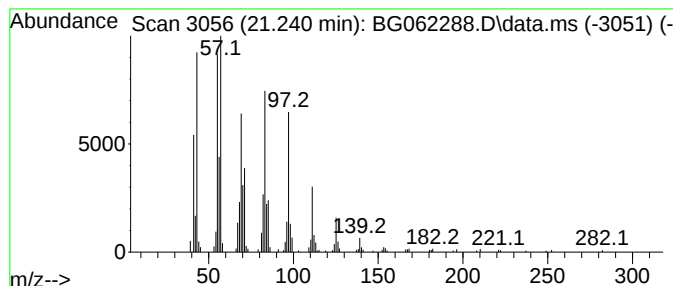
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 E-15-Heptadecenal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.240	6.34 ng/ul	344049	Chrysene-d12	21.558

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal			252	C17H32O	1000130-97-9	96
2	1-Docosene			308	C22H44	001599-67-3	95
3	1-Nonadecene			266	C19H38	018435-45-5	91
4	1-Hexacosene			364	C26H52	018835-33-1	91
5	2- Chloropropionic acid, octadec...			360	C21H41ClO2	088104-31-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
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Operator : MA/JU
Sample : P3336-07
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.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
Propylene Glycol	3.682	8.4	ng/ul	125590	1	7.958	300236	20.0
Pentanedioic ac...	9.674	2.2	ng/ul	54206	2	10.755	501956	20.0
1-Phenoxypropan...	11.489	5.4	ng/ul	135018	2	10.755	501956	20.0
unknown-01	14.808	3.1	ng/ul	120542	3	14.579	788476	20.0
n-Hexadecanoic ...	18.221	4.9	ng/ul	236037	4	17.316	955624	20.0
E-15-Heptadecenal	21.240	6.3	ng/ul	344049	5	21.558	1085990	20.0