

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
 Data File : BG062261.D
 Acq On : 6 Aug 2024 7:49
 Operator : MA/JU
 Sample : P3361-16
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 E20P6

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: BG062261.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.424	20	23	29	rVB3	9322	12600	0.70%	0.063%
2	3.682	63	67	80	rBV	49235	78170	4.32%	0.392%
3	3.829	87	92	106	rBV	140472	233899	12.91%	1.174%
4	4.176	147	151	155	rVB5	3345	4893	0.27%	0.025%
5	4.299	169	172	176	rBV3	1662	2300	0.13%	0.012%
6	4.822	258	261	264	rBV3	1944	2789	0.15%	0.014%
7	5.069	301	303	311	rVB7	1527	3524	0.19%	0.018%
8	6.050	465	470	474	rBV3	4978	6925	0.38%	0.035%
9	6.937	616	621	624	rBV4	1837	2691	0.15%	0.014%
10	7.113	644	651	660	rBV	217568	365129	20.16%	1.833%
11	7.289	675	681	689	rBV	150048	251971	13.91%	1.265%
12	7.495	709	716	722	rBV	192766	328038	18.11%	1.647%
13	7.553	722	726	735	rVB	29416	46312	2.56%	0.233%
14	7.965	788	796	803	rBV	216321	356084	19.66%	1.788%
15	8.023	803	806	813	rVB2	5293	7259	0.40%	0.036%
16	8.652	904	913	923	rBV	273107	472342	26.08%	2.371%
17	9.116	982	992	1003	rBV	191075	341660	18.86%	1.715%
18	9.222	1007	1010	1017	rVB4	1895	3443	0.19%	0.017%
19	9.292	1019	1022	1025	rBV3	1346	1816	0.10%	0.009%
20	9.580	1064	1071	1074	rBV2	2280	3634	0.20%	0.018%
21	9.680	1082	1088	1093	rBV2	22673	35336	1.95%	0.177%
22	9.833	1106	1114	1123	rBV	145863	256658	14.17%	1.289%
23	10.367	1197	1205	1214	rBV	280864	495772	27.37%	2.489%
24	10.761	1264	1272	1280	rVB	331510	598405	33.04%	3.004%
25	10.884	1284	1293	1306	rBV	288664	510820	28.20%	2.564%
26	11.219	1347	1350	1354	rBV2	1447	1917	0.11%	0.010%
27	11.295	1356	1363	1367	rBV2	11029	16179	0.89%	0.081%
28	11.495	1391	1397	1411	rVB	95465	171051	9.44%	0.859%
29	11.695	1427	1431	1437	rVB4	1118	1815	0.10%	0.009%
30	12.235	1519	1523	1527	rVB3	1834	2943	0.16%	0.015%
31	12.341	1536	1541	1545	rBV2	4607	6928	0.38%	0.035%
32	12.946	1640	1644	1645	rBV2	2053	1888	0.10%	0.009%
33	12.958	1645	1646	1650	rVB2	2207	1894	0.10%	0.010%
34	13.152	1675	1679	1682	rBV2	1419	2191	0.12%	0.011%
35	13.199	1682	1687	1691	rBV3	2628	4072	0.22%	0.020%
36	13.428	1723	1726	1733	rVB2	4597	7418	0.41%	0.037%

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Integrator: RTE

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37	13.492	1733	1737	1740	rBV3	1025	1867	0.10%	0.009%
38	13.569	1742	1750	1754	rVB4	4602	7164	0.40%	0.036%
39	13.786	1783	1787	1789	rBV2	1584	2052	0.11%	0.010%
40	13.804	1789	1790	1795	rVB3	1557	1947	0.11%	0.010%
41	13.992	1815	1822	1828	rBV	612996	860343	47.50%	4.319%
42	14.045	1828	1831	1833	rVV	2313	2719	0.15%	0.014%
43	14.274	1859	1870	1878	rBV	666114	1086183	59.97%	5.453%
44	14.503	1904	1909	1914	rVB3	4751	6307	0.35%	0.032%
45	14.585	1914	1923	1930	rBV	630350	970620	53.59%	4.873%
46	14.755	1944	1952	1956	rBV	255968	411876	22.74%	2.068%
47	14.797	1956	1959	1960	rBV	114360	120091	6.63%	0.603%
48	14.996	1989	1993	1999	rBV4	4165	4817	0.27%	0.024%
49	15.084	2006	2008	2012	rBV2	3059	4005	0.22%	0.020%
50	15.396	2055	2061	2066	rVB3	5546	10437	0.58%	0.052%
51	15.449	2066	2070	2075	rBV3	6194	8906	0.49%	0.045%
52	15.578	2083	2092	2099	rBV	905491	1392959	76.91%	6.993%
53	15.678	2103	2109	2115	rBV	156916	224074	12.37%	1.125%
54	15.754	2119	2122	2124	rVB3	2682	3116	0.17%	0.016%
55	15.813	2129	2132	2137	rVV5	3460	6260	0.35%	0.031%
56	15.860	2137	2140	2148	rVV5	2944	5989	0.33%	0.030%
57	15.942	2150	2154	2156	rVV3	2110	2933	0.16%	0.015%
58	15.960	2156	2157	2161	rVV2	1890	1985	0.11%	0.010%
59	16.013	2161	2166	2172	rVB6	3371	5257	0.29%	0.026%
60	16.130	2182	2186	2193	rBV2	12752	17980	0.99%	0.090%
61	16.259	2205	2208	2211	rBV5	1861	2398	0.13%	0.012%
62	16.312	2211	2217	2220	rVV3	9200	14255	0.79%	0.072%
63	16.342	2220	2222	2227	rVB5	6535	8003	0.44%	0.040%
64	16.477	2244	2245	2249	rVB4	2598	2667	0.15%	0.013%
65	16.588	2260	2264	2266	rBV4	1700	2453	0.14%	0.012%
66	16.647	2273	2274	2278	rBV4	2297	2610	0.14%	0.013%
67	16.676	2278	2279	2283	rBV4	1436	2232	0.12%	0.011%
68	16.823	2298	2304	2308	rBV7	1921	3410	0.19%	0.017%
69	16.894	2312	2316	2321	rBV4	6739	9517	0.53%	0.048%
70	17.058	2340	2344	2346	rVB4	4099	4081	0.23%	0.020%
71	17.105	2346	2352	2356	rBV4	8441	12821	0.71%	0.064%
72	17.158	2359	2361	2367	rVB6	3935	4549	0.25%	0.023%
73	17.258	2372	2378	2381	rVB6	3846	8691	0.48%	0.044%
74	17.323	2382	2389	2396	rVV	795593	1204227	66.49%	6.046%
75	17.422	2399	2406	2413	rBV	968217	1446407	79.86%	7.261%
76	17.505	2418	2420	2423	rVB4	3412	3520	0.19%	0.018%

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77	17.652	2442	2445	2449	rBV6	4216	5474	0.30%	0.027%
78	17.687	2449	2451	2453	rBV3	2927	2485	0.14%	0.012%
79	17.722	2453	2457	2460	rVB6	7697	10001	0.55%	0.050%
80	17.751	2460	2462	2464	rBV3	1825	2146	0.12%	0.011%
81	17.845	2474	2478	2481	rBV3	6676	9542	0.53%	0.048%
82	18.010	2502	2506	2513	rVB2	32784	42491	2.35%	0.213%
83	18.233	2538	2544	2558	rBV	193133	330633	18.26%	1.660%
84	18.539	2593	2596	2601	rBV6	9909	10417	0.58%	0.052%
85	18.997	2672	2674	2676	rBV3	5333	4192	0.23%	0.021%
86	19.091	2687	2690	2696	rVB8	19615	31632	1.75%	0.159%
87	19.179	2701	2705	2709	rVB4	48728	59206	3.27%	0.297%
88	19.267	2717	2720	2725	rBV3	14602	20144	1.11%	0.101%
89	19.337	2730	2732	2737	rVB4	11976	18560	1.02%	0.093%
90	19.502	2755	2760	2767	rBV	92691	145867	8.05%	0.732%
91	19.702	2788	2794	2802	rVV	1246681	1764812	97.44%	8.860%
92	19.772	2802	2806	2811	rVB3	30144	36735	2.03%	0.184%
93	21.247	3053	3057	3066	rVB	200736	282590	15.60%	1.419%
94	21.564	3105	3111	3118	rVB	802524	1271687	70.21%	6.384%
95	23.861	3498	3502	3510	rBV2	30724	66385	3.67%	0.333%
96	24.448	3593	3602	3616	rVB	673559	1811139	100.00%	9.092%
97	24.660	3628	3638	3649	rBV	519731	1386946	76.58%	6.963%
98	24.783	3657	3659	3669	rVB4	37231	73480	4.06%	0.369%

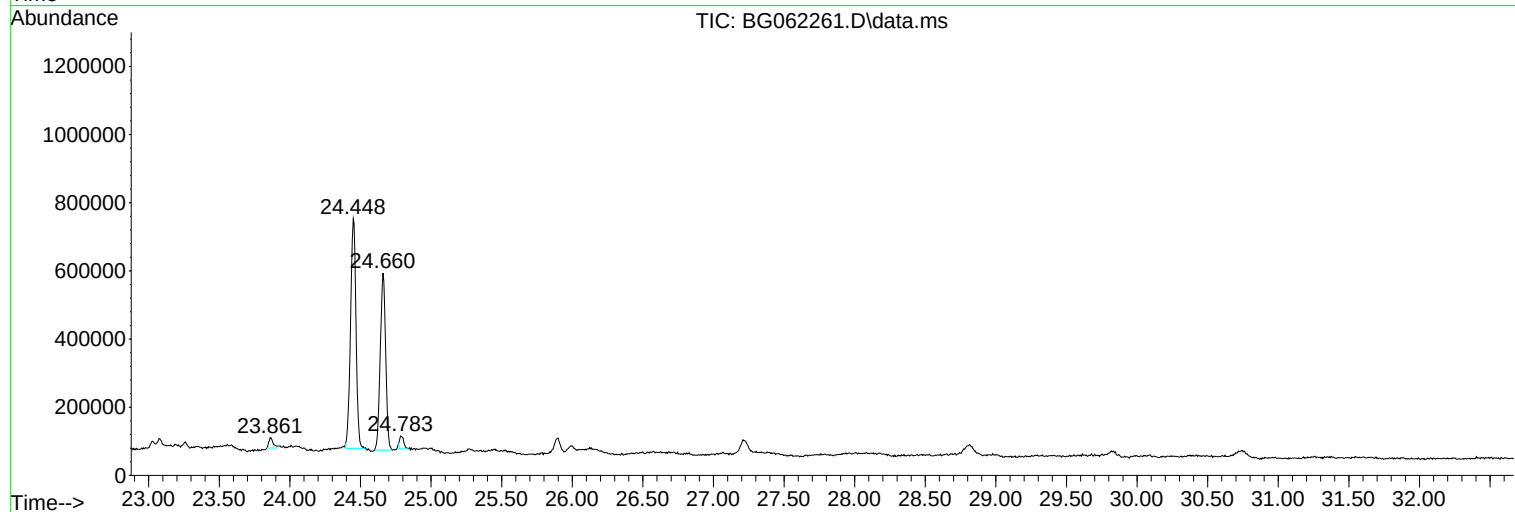
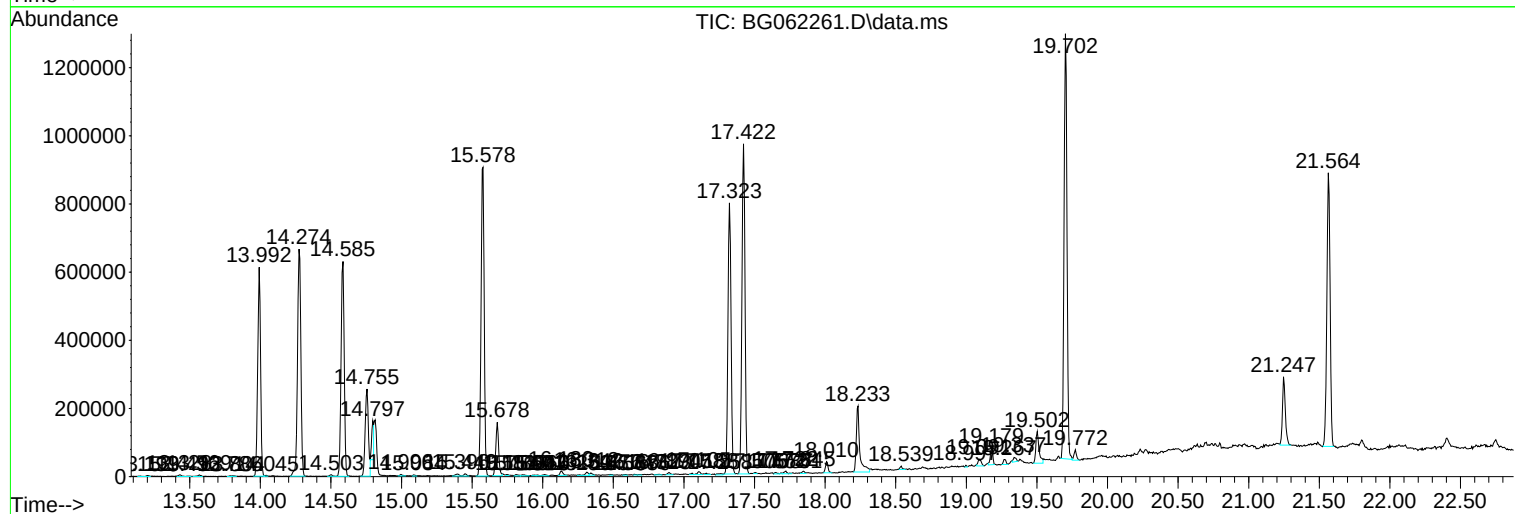
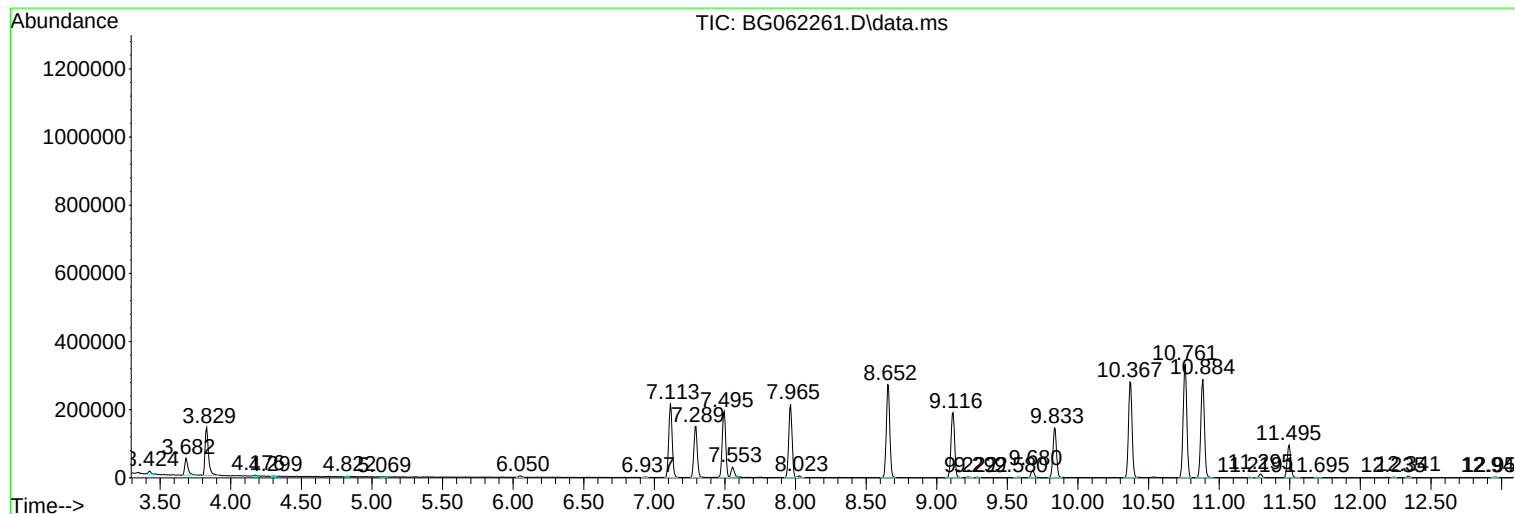
Sum of corrected areas: 19919058

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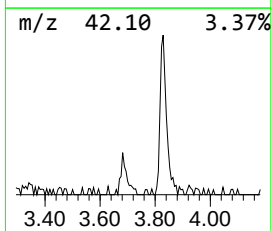
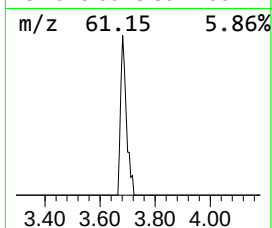
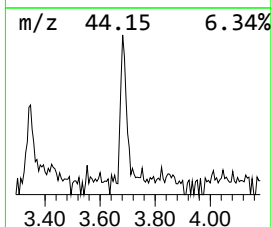
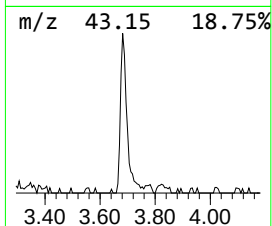
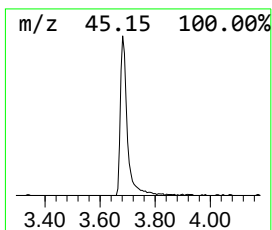
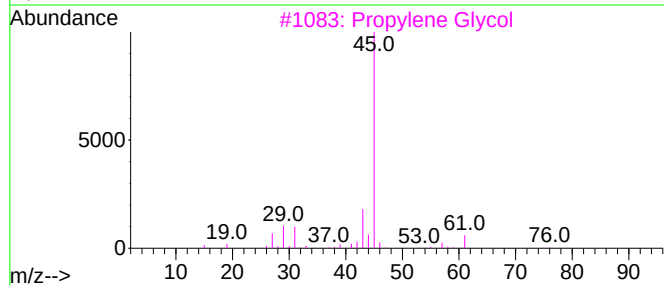
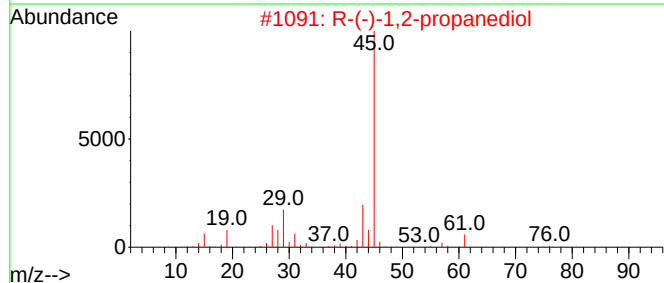
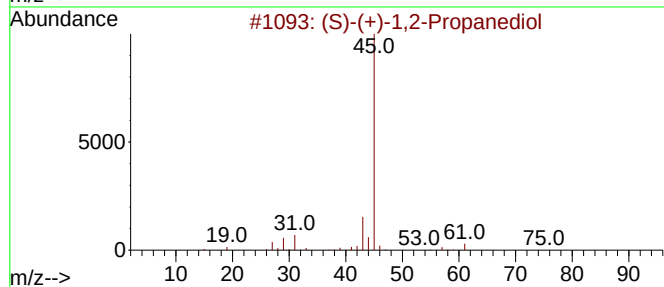
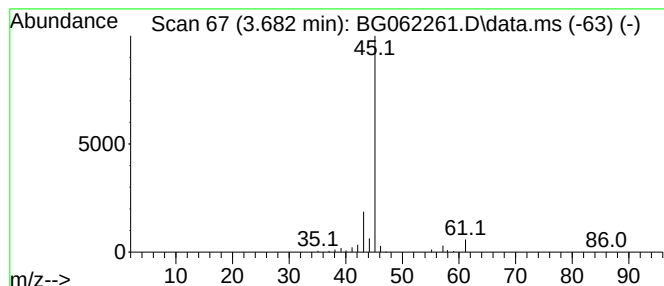
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.682	4.39 ng/ul	78170	1,4-Dichlorobenzene-d4	7.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	43
3	Propylene Glycol			76	C3H8O2	000057-55-6	43
4	4-Penten-2-ol			86	C5H10O	000625-31-0	39
5	Propylene Glycol			76	C3H8O2	000057-55-6	9



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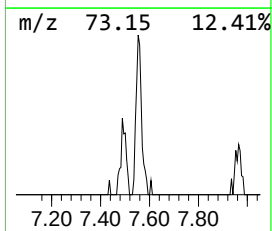
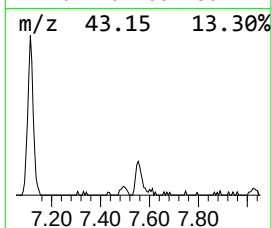
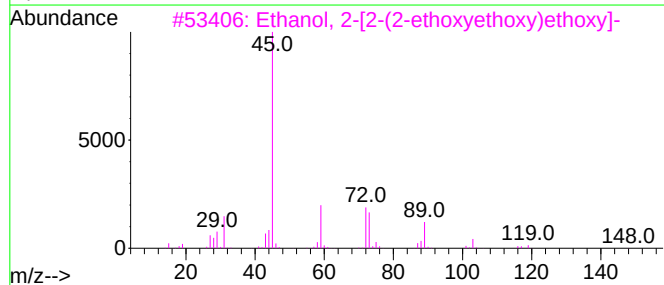
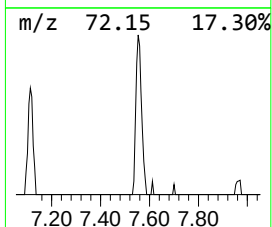
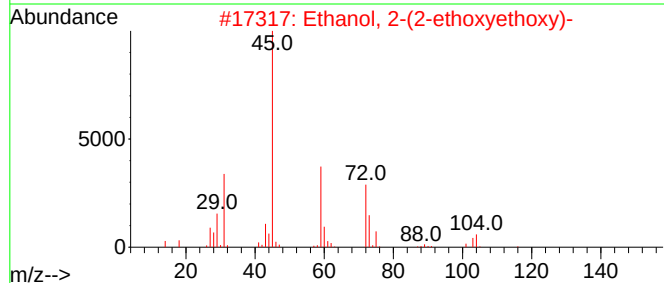
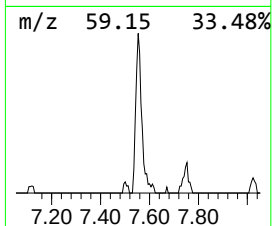
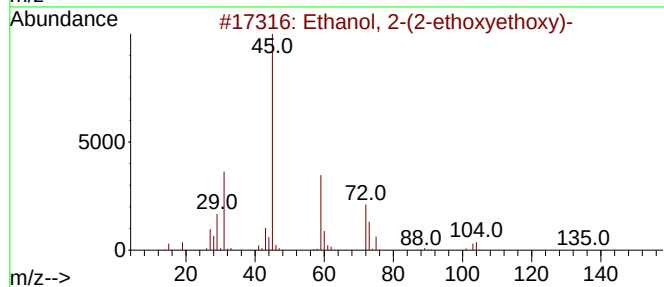
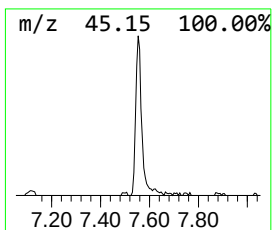
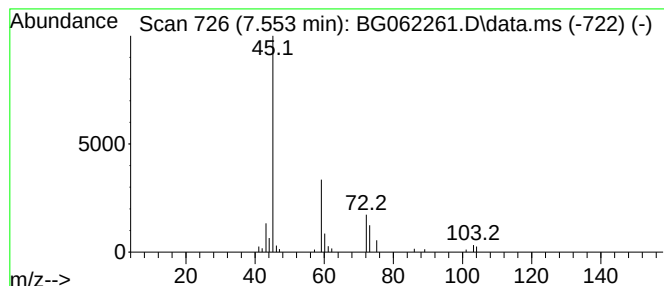
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.553	2.60 ng/ul	46312	1,4-Dichlorobenzene-d4	7.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	64
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	56
4			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	47
5			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	40



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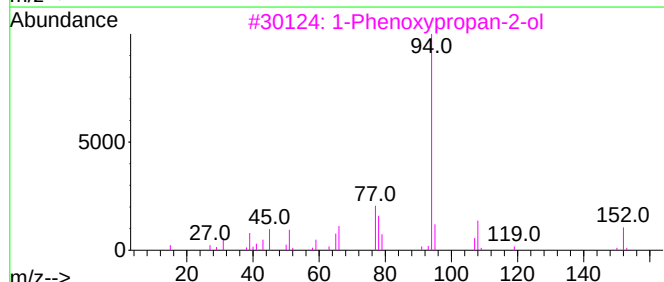
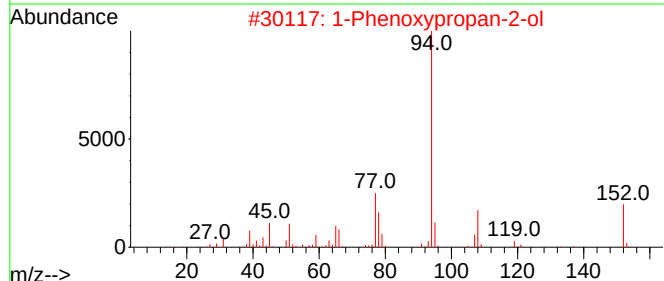
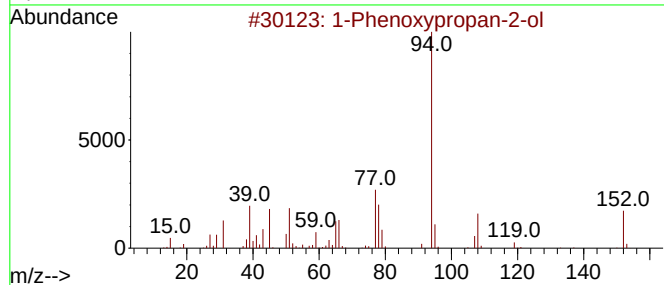
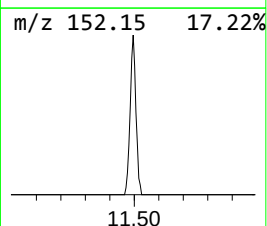
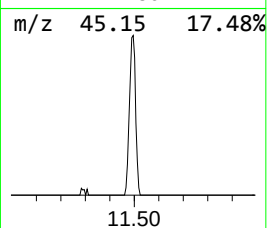
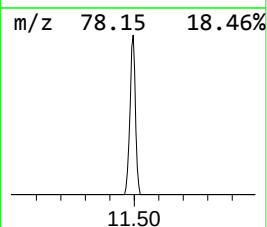
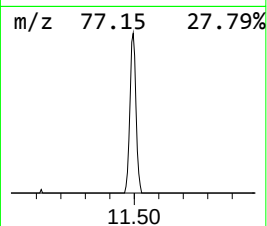
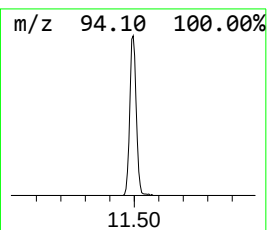
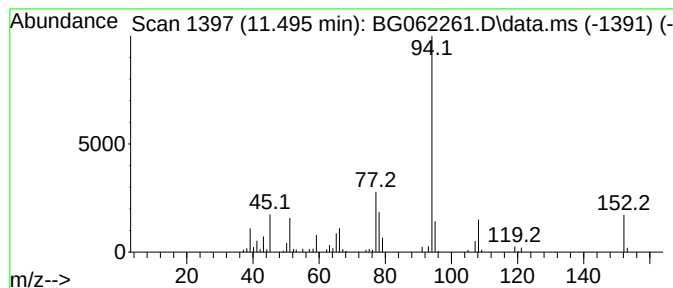
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.495	5.72 ng/ul	171051	Naphthalene-d8	10.761

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
3			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
4			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
5			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062261.D
Acq On : 6 Aug 2024 7:49
Operator : MA/JU
Sample : P3361-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P6

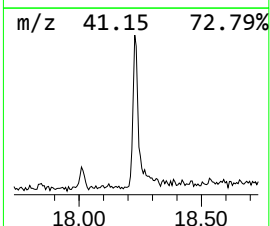
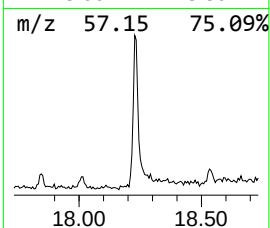
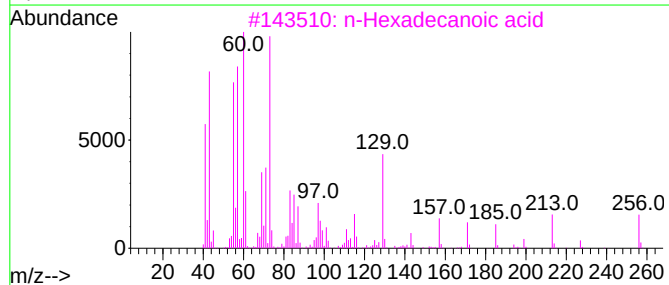
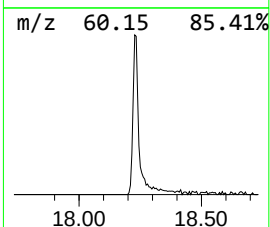
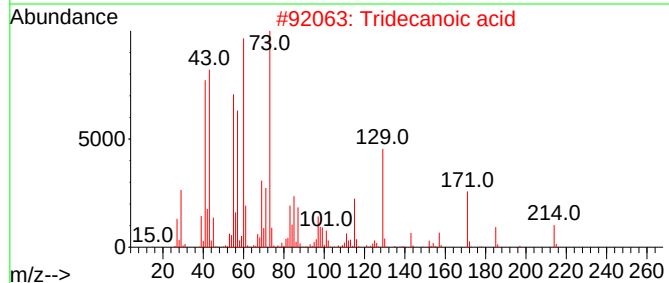
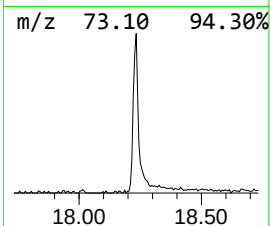
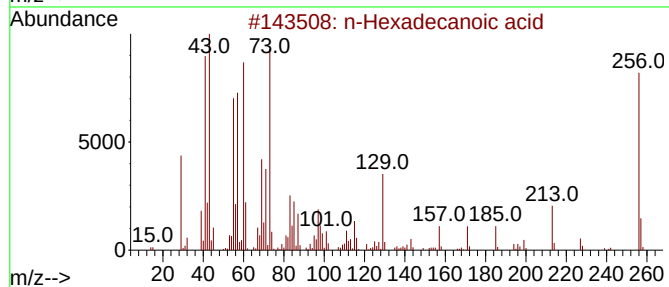
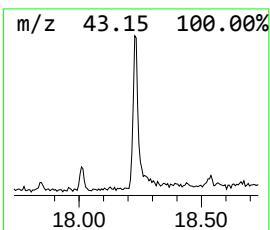
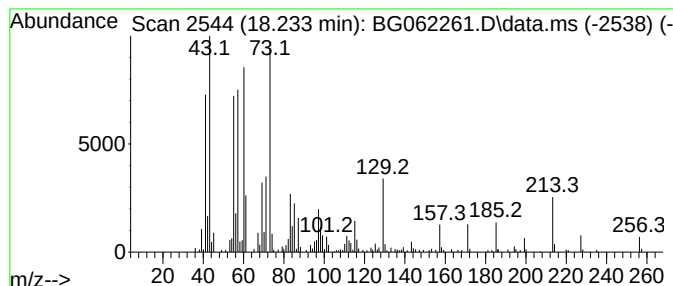
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	5.49 ng/ul	330633	Phenanthrene-d10	17.323

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4			Tridecanoic acid	214	C13H26O2	000638-53-9	89
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062261.D
Acq On : 6 Aug 2024 7:49
Operator : MA/JU
Sample : P3361-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P6

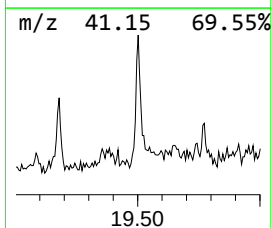
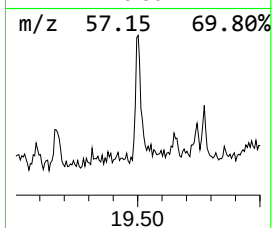
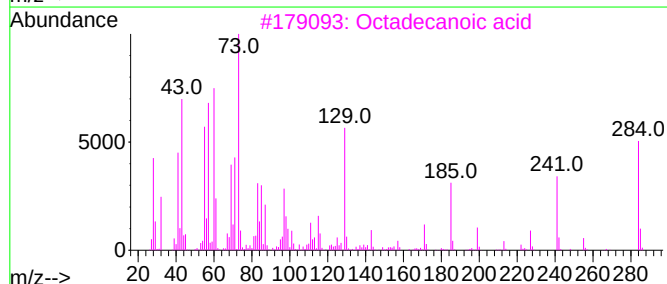
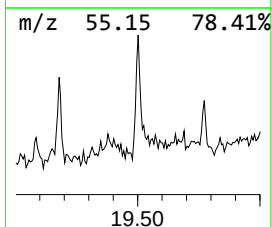
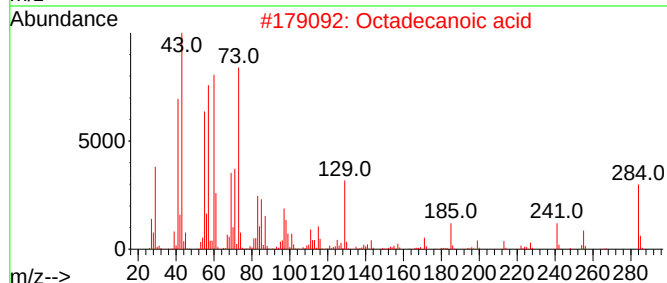
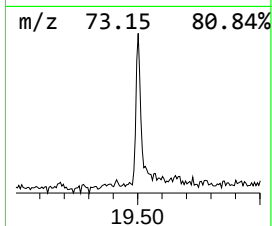
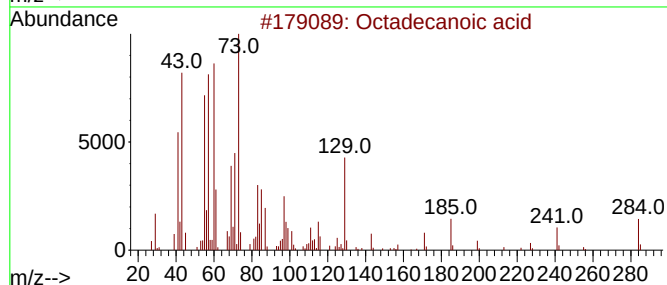
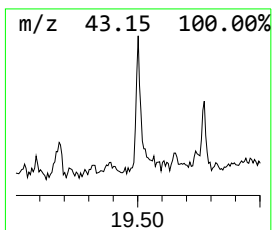
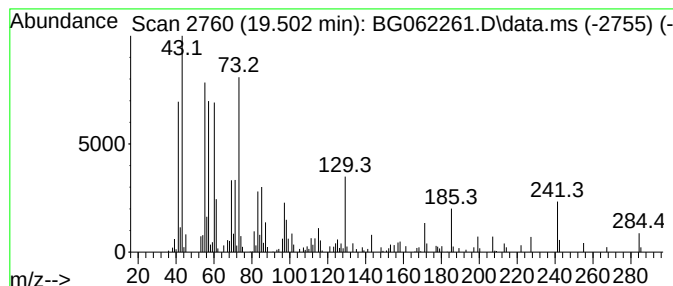
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.502	2.29 ng/ul	145867	Chrysene-d12	21.564

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Octadecanoic acid	284	C18H36O2	000057-11-4	92
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062261.D
Acq On : 6 Aug 2024 7:49
Operator : MA/JU
Sample : P3361-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P6

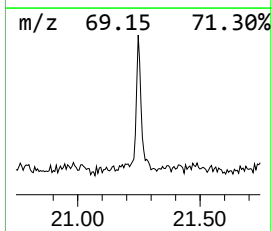
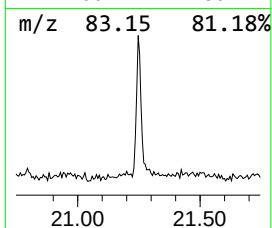
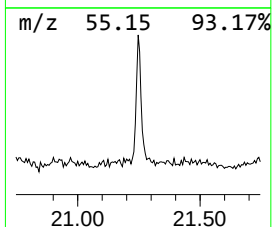
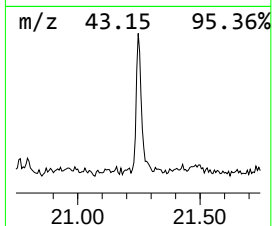
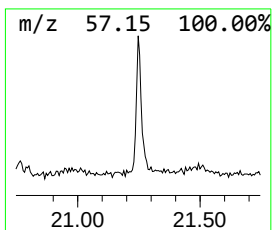
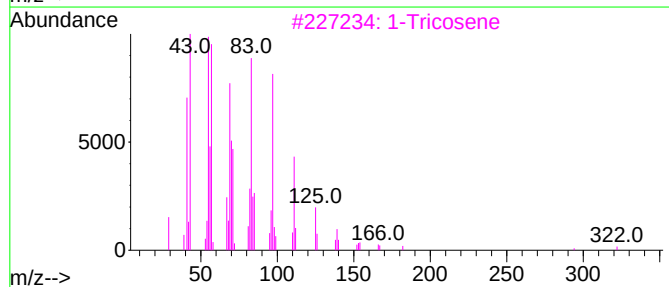
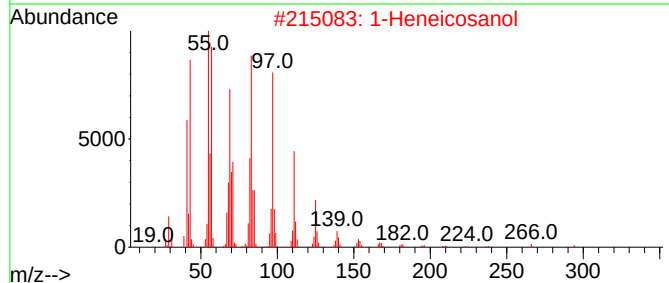
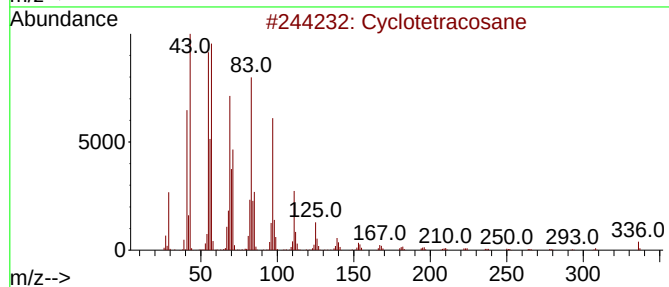
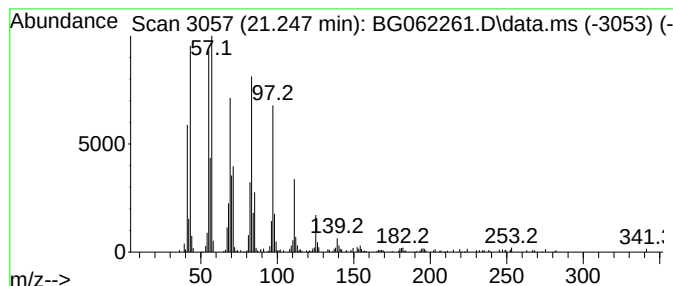
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Cyclic21.247 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.247	4.44 ng/ul	282590	Chrysene-d12	21.564

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	91
2			1-Heneicosanol	312	C21H44O	015594-90-8	91
3			1-Tricosene	322	C23H46	018835-32-0	91
4			Octacosanol	410	C28H58O	000557-61-9	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062261.D
Acq On : 6 Aug 2024 7:49
Operator : MA/JU
Sample : P3361-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P6

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
(S)-(+)-1,2-Pro...	3.682	4.4	ng/ul	78170	1	7.965	356084	20.0
Ethanol, 2-(2-e...	7.553	2.6	ng/ul	46312	1	7.965	356084	20.0
1-Phenoxypropan...	11.495	5.7	ng/ul	171051	2	10.761	598405	20.0
n-Hexadecanoic ...	18.233	5.5	ng/ul	330633	4	17.323	1204230	20.0
Octadecanoic acid	19.502	2.3	ng/ul	145867	5	21.564	1271690	20.0
(DEL) Alkane: C...	21.247	4.4	ng/ul	282590	5	21.564	1271690	20.0