

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
 Data File : BG062542.D
 Acq On : 22 Aug 2024 16:04
 Operator : MA/JU
 Sample : P3673-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DCYD1

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-BG081424.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG062542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.406	16	20	25	rVB3	9438	12369	0.86%	0.074%
2	3.664	60	64	71	rBV	29970	45070	3.12%	0.269%
3	3.811	85	89	98	rBV	36705	61646	4.27%	0.367%
4	4.040	126	128	133	rVB5	2195	2656	0.18%	0.016%
5	4.146	142	146	149	rBV4	5072	6689	0.46%	0.040%
6	5.051	296	300	302	rBV3	2352	2737	0.19%	0.016%
7	6.020	460	465	473	rBV2	7380	12494	0.87%	0.074%
8	6.202	491	496	501	rBV4	1400	2230	0.15%	0.013%
9	6.637	565	570	576	rVB3	5347	7722	0.54%	0.046%
10	6.919	614	618	622	rVB5	1766	2628	0.18%	0.016%
11	7.101	642	649	657	rBV	162685	277109	19.20%	1.651%
12	7.265	671	677	685	rBV	113038	181685	12.59%	1.083%
13	7.471	703	712	719	rBV	139452	237771	16.48%	1.417%
14	7.530	719	722	726	rVB3	4911	7232	0.50%	0.043%
15	7.935	784	791	798	rBV	242060	396345	27.46%	2.362%
16	8.000	798	802	806	rVB4	4590	7997	0.55%	0.048%
17	8.634	903	910	918	rBV	196884	339641	23.53%	2.024%
18	9.086	979	987	997	rBV	137599	244494	16.94%	1.457%
19	9.521	1056	1061	1063	rBV4	2095	2598	0.18%	0.015%
20	9.650	1073	1083	1092	rBV2	21726	36463	2.53%	0.217%
21	9.809	1103	1110	1118	rBV	116599	199578	13.83%	1.189%
22	10.038	1142	1149	1154	rVB6	2731	5829	0.40%	0.035%
23	10.349	1193	1202	1212	rBV	205153	362978	25.15%	2.163%
24	10.731	1259	1267	1277	rVB	350859	627796	43.50%	3.741%
25	10.861	1281	1289	1299	rBV	164562	307515	21.31%	1.832%
26	11.031	1313	1318	1322	rVB2	3134	4371	0.30%	0.026%
27	11.254	1352	1356	1363	rVV3	9349	14957	1.04%	0.089%
28	11.466	1384	1392	1402	rBV	41514	83503	5.79%	0.498%
29	12.306	1529	1535	1540	rBV2	3862	6133	0.42%	0.037%
30	13.169	1678	1682	1686	rBV2	1297	2183	0.15%	0.013%
31	13.392	1715	1720	1724	rBV3	3815	5335	0.37%	0.032%
32	13.962	1811	1817	1826	rBV	422615	593736	41.14%	3.538%
33	14.250	1854	1866	1873	rVV	475841	730738	50.64%	4.354%
34	14.462	1899	1902	1906	rVB4	2023	3140	0.22%	0.019%
35	14.561	1912	1919	1927	rVB	640977	1046315	72.50%	6.234%
36	14.749	1945	1951	1962	rBV2	193638	356542	24.71%	2.124%

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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
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37	14.973	1984	1989	1993	rBV3	4359	7234	0.50%	0.043%
38	15.149	2014	2019	2021	rBV3	1832	3101	0.21%	0.018%
39	15.354	2051	2054	2059	rBV3	3602	5651	0.39%	0.034%
40	15.413	2059	2064	2068	rBV4	2996	4352	0.30%	0.026%

41	15.548	2080	2087	2095	rBV	659842	1008988	69.92%	6.012%
42	15.660	2099	2106	2112	rBV	179256	262483	18.19%	1.564%
43	15.713	2112	2115	2117	rVB3	1683	2204	0.15%	0.013%
44	15.783	2124	2127	2132	rBV4	3024	4807	0.33%	0.029%
45	15.983	2159	2161	2165	rVV5	2794	2429	0.17%	0.014%

46	16.095	2178	2180	2183	rBV3	2795	3485	0.24%	0.021%
47	16.277	2204	2211	2214	rBV5	5182	8480	0.59%	0.051%
48	16.412	2230	2234	2236	rBV3	3156	3600	0.25%	0.021%
49	16.435	2236	2238	2244	rVV4	2123	3440	0.24%	0.020%
50	16.529	2248	2254	2256	rVB4	1356	2417	0.17%	0.014%

51	16.700	2279	2283	2286	rBV2	3015	3522	0.24%	0.021%
52	16.729	2286	2288	2293	rVB4	2461	4009	0.28%	0.024%
53	16.805	2296	2301	2305	rVB6	4931	6411	0.44%	0.038%
54	16.864	2305	2311	2314	rBV4	5679	8825	0.61%	0.053%
55	17.017	2333	2337	2341	rBV4	3963	5058	0.35%	0.030%

56	17.070	2341	2346	2349	rBV5	4187	6466	0.45%	0.039%
57	17.199	2362	2368	2371	rBV4	3340	6399	0.44%	0.038%
58	17.228	2371	2373	2375	rVV2	3196	2749	0.19%	0.016%
59	17.299	2375	2385	2394	rVV	930673	1390830	96.38%	8.287%
60	17.399	2395	2402	2412	rVV2	751990	1128709	78.21%	6.725%

61	17.487	2412	2417	2424	rVV7	3755	10460	0.72%	0.062%
62	17.546	2424	2427	2429	rVV2	3290	3576	0.25%	0.021%
63	17.587	2431	2434	2437	rVV4	4828	6517	0.45%	0.039%
64	17.804	2468	2471	2475	rBV5	4044	5971	0.41%	0.036%
65	17.869	2479	2482	2483	rVV3	2401	2661	0.18%	0.016%

66	17.880	2483	2484	2488	rVV3	3109	2359	0.16%	0.014%
67	17.927	2490	2492	2495	rVB3	2437	2692	0.19%	0.016%
68	17.974	2495	2500	2503	rBV4	9784	10511	0.73%	0.063%
69	18.057	2512	2514	2515	rBV2	2759	2294	0.16%	0.014%
70	18.198	2533	2538	2548	rBV2	91747	168323	11.66%	1.003%

71	18.497	2586	2589	2592	rVB4	3618	4348	0.30%	0.026%
72	18.738	2627	2630	2631	rBV2	2713	2691	0.19%	0.016%
73	18.826	2642	2645	2648	rVV5	5841	6526	0.45%	0.039%
74	18.920	2659	2661	2664	rBV4	3921	3518	0.24%	0.021%
75	19.067	2682	2686	2688	rBV4	3158	4369	0.30%	0.026%

76	19.114	2692	2694	2697	rVV4	3519	4116	0.29%	0.025%
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77	19.196	2707	2708	2713	rBV5	2251	3023	0.21%	0.018%
78	19.249	2713	2717	2722	rVB6	10922	17554	1.22%	0.105%
79	19.326	2723	2730	2733	rBV2	15756	26088	1.81%	0.155%
80	19.472	2750	2755	2760	rBV4	31210	46217	3.20%	0.275%
81	19.625	2777	2781	2785	rBV6	12745	15827	1.10%	0.094%
82	19.684	2785	2791	2798	rVV	900336	1301222	90.17%	7.753%
83	19.737	2798	2800	2806	rVB3	15599	20047	1.39%	0.119%
84	20.130	2864	2867	2873	rBV8	5979	11681	0.81%	0.070%
85	20.201	2876	2879	2882	rBV4	8253	12536	0.87%	0.075%
86	20.230	2882	2884	2889	rVV3	11760	15582	1.08%	0.093%
87	20.295	2893	2895	2896	rBV2	4580	3698	0.26%	0.022%
88	20.606	2944	2948	2952	rVB2	29550	34925	2.42%	0.208%
89	20.665	2954	2958	2962	rBV4	16598	22205	1.54%	0.132%
90	21.035	3017	3021	3026	rVB	52671	69212	4.80%	0.412%
91	21.217	3047	3052	3060	rBV	114894	196547	13.62%	1.171%
92	21.546	3102	3108	3121	rBV	862092	1367964	94.79%	8.151%
93	21.752	3141	3143	3149	rVB4	16521	20872	1.45%	0.124%
94	22.363	3240	3247	3258	rBV6	46097	144858	10.04%	0.863%
95	23.191	3384	3388	3394	rVB2	28197	50418	3.49%	0.300%
96	23.778	3483	3488	3494	rVB3	42440	82584	5.72%	0.492%
97	24.419	3588	3597	3609	rVB	435398	1145190	79.35%	6.823%
98	24.636	3624	3634	3648	rVB2	511021	1443137	100.00%	8.599%
99	25.758	3818	3825	3835	rVB7	41029	114691	7.95%	0.683%
100	25.876	3837	3845	3858	rVV3	72566	252579	17.50%	1.505%

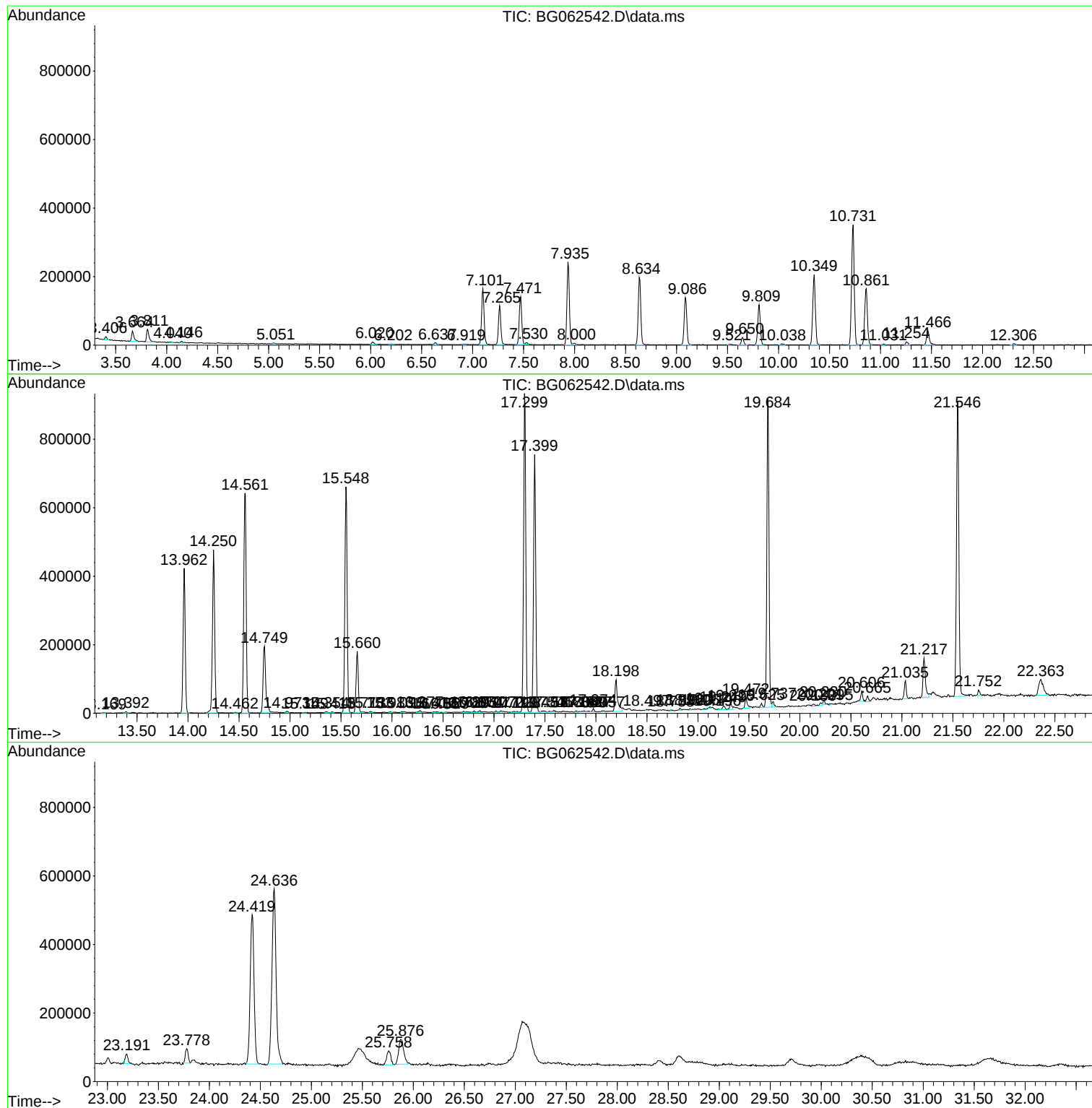
Sum of corrected areas: 16783463

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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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



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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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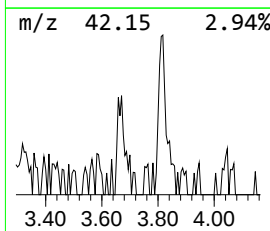
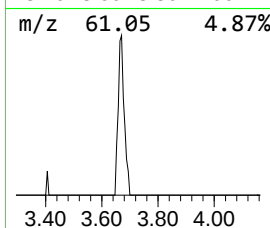
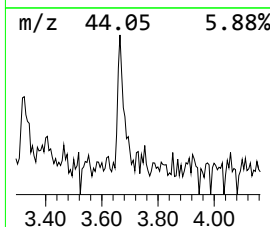
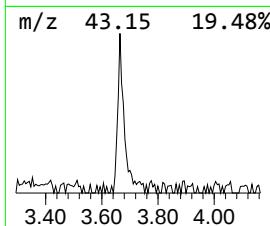
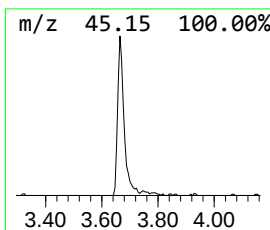
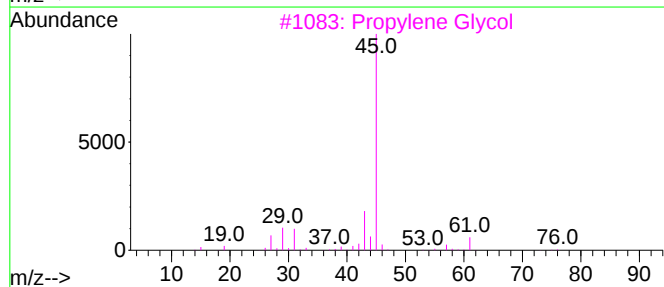
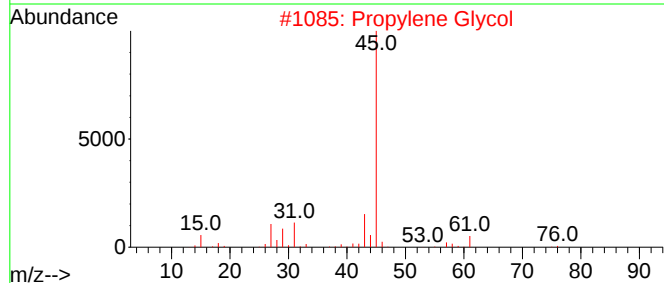
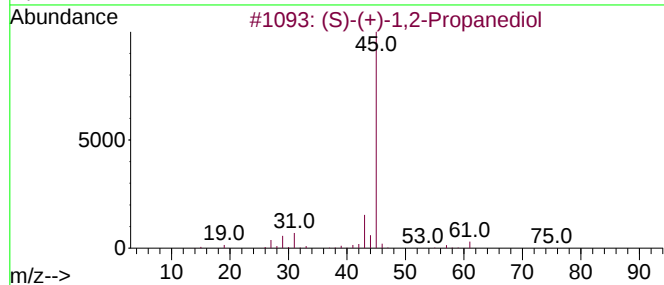
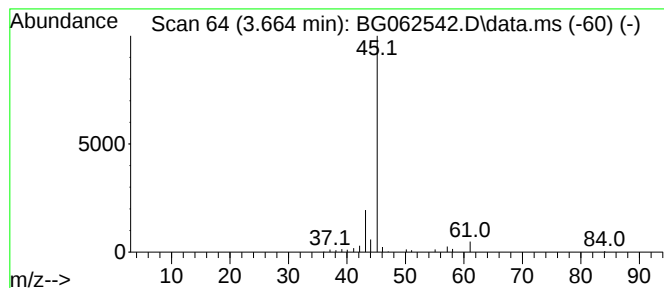
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.664	2.27 ng/ul	45070	1,4-Dichlorobenzene-d4	7.935

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	56
2	Propylene Glycol			76	C3H8O2	000057-55-6	43
3	Propylene Glycol			76	C3H8O2	000057-55-6	43
4	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	40
5	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	40



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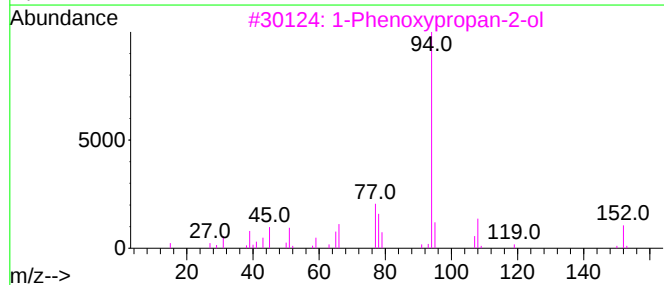
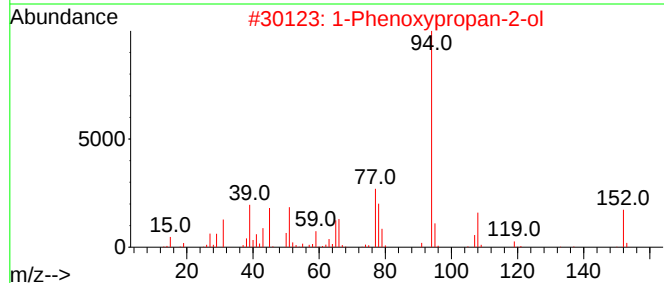
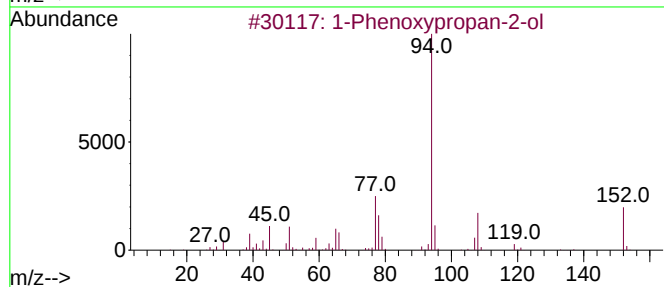
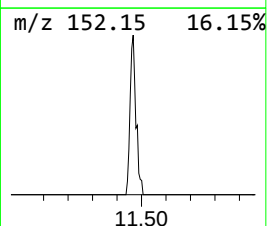
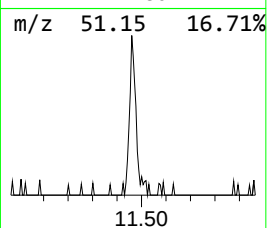
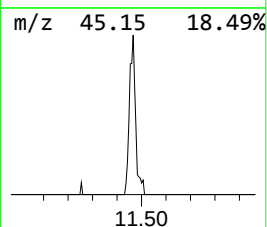
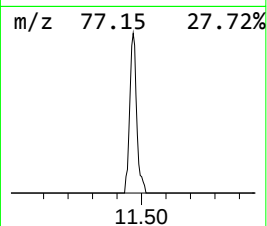
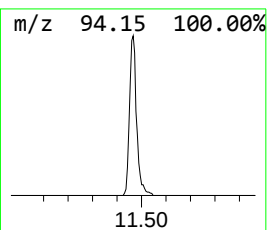
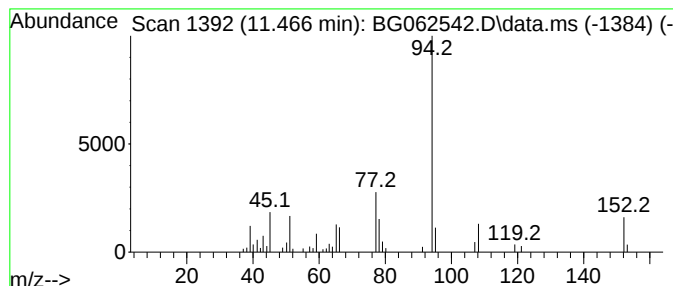
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.466	2.66 ng/ul	83503	Naphthalene-d8	10.731

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	90
4			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	90
5			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	90



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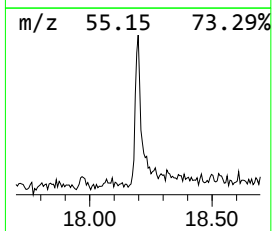
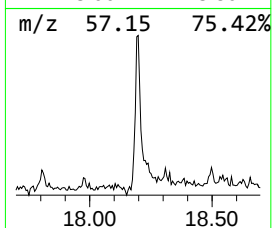
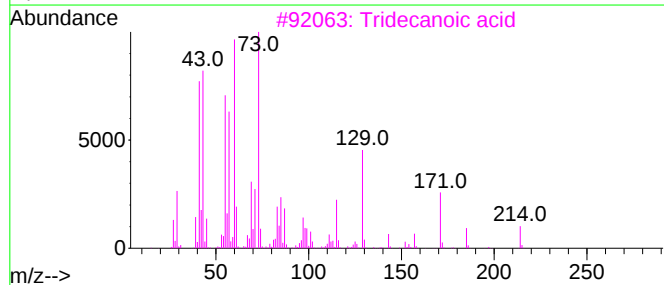
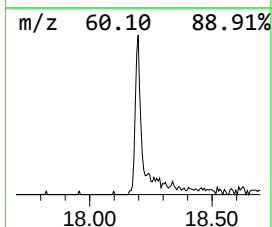
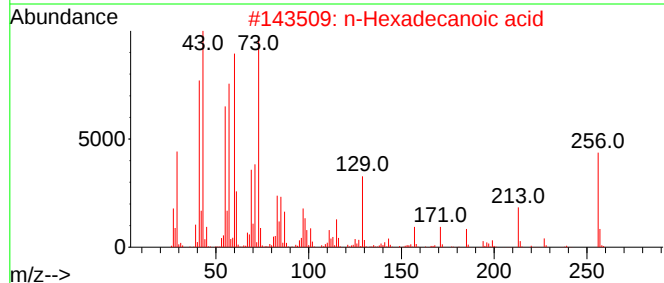
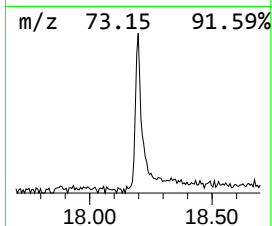
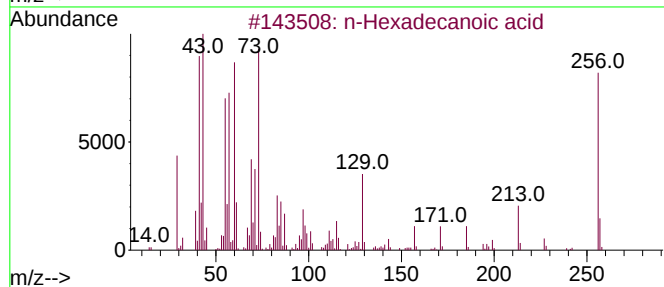
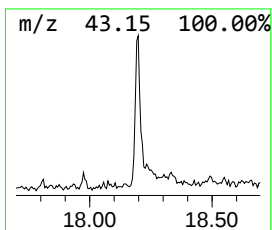
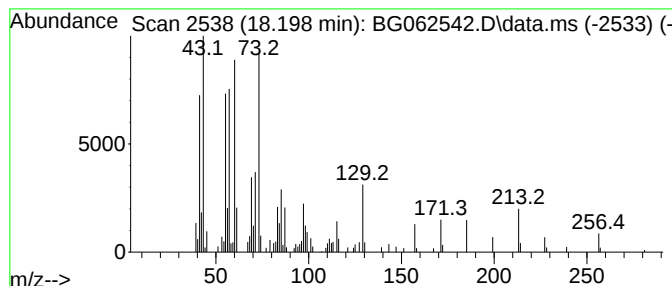
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	2.42 ng/ul	168323	Phenanthrene-d10	17.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062542.D
Acq On : 22 Aug 2024 16:04
Operator : MA/JU
Sample : P3673-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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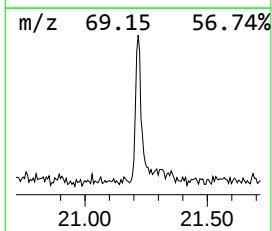
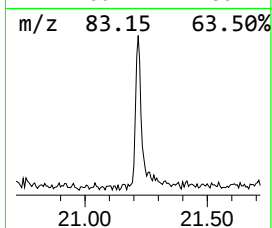
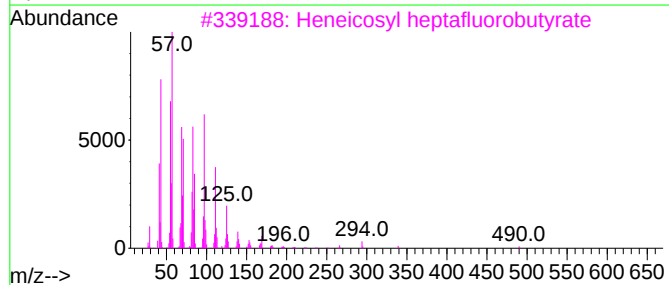
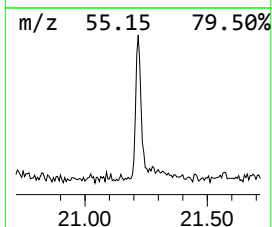
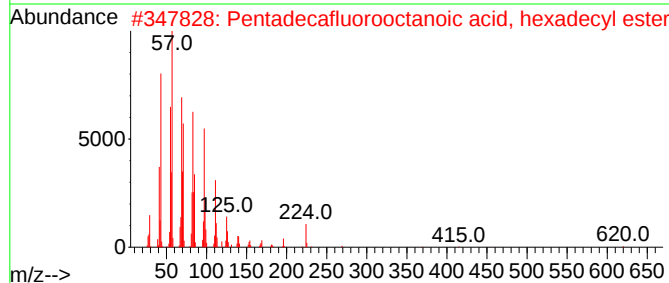
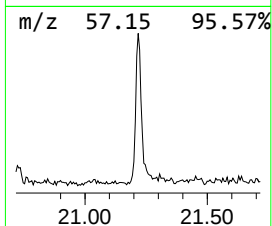
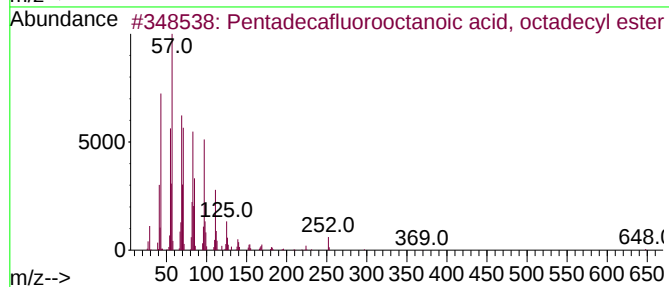
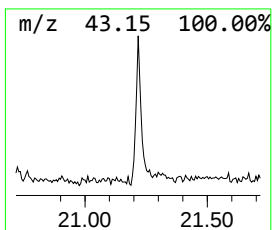
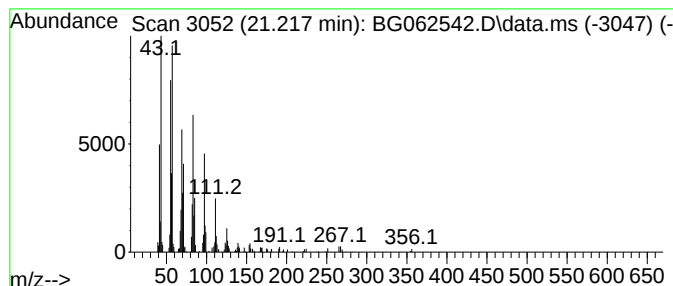
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.217	2.87 ng/ul	196547	Chrysene-d12	21.546

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	91
3			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5			Cyclotetracosane	336	C24H48	000297-03-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062542.D
Acq On : 22 Aug 2024 16:04
Operator : MA/JU
Sample : P3673-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD1

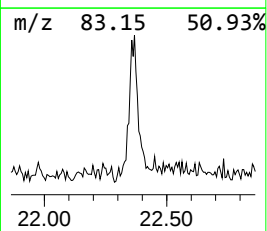
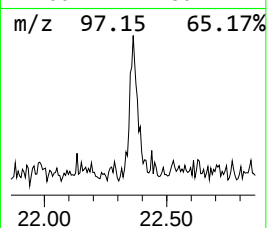
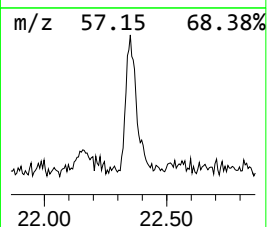
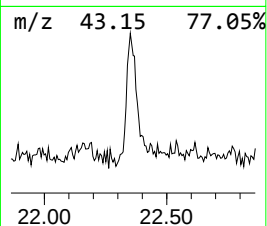
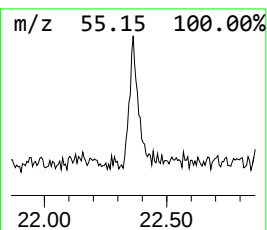
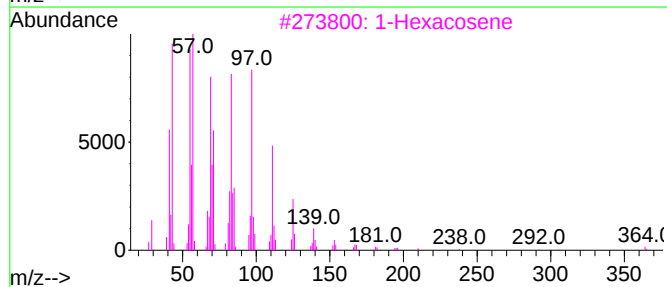
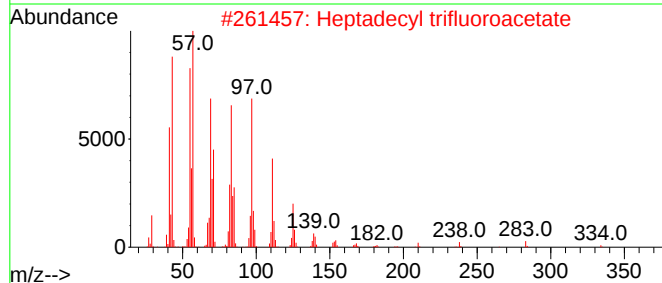
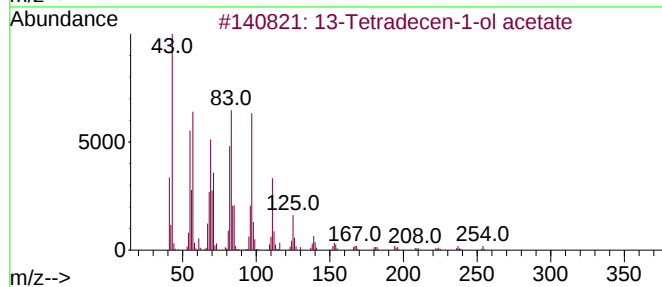
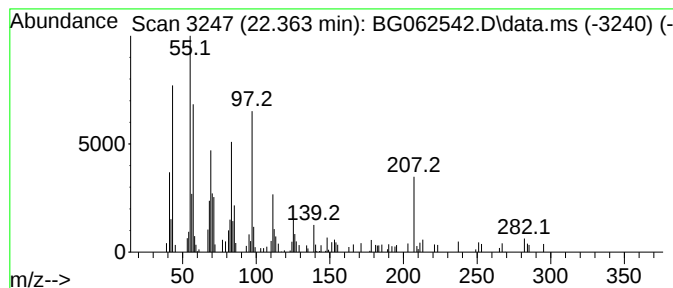
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 13-Tetradecen-1-ol acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.363	2.12 ng/ul	144858	Chrysene-d12	21.546

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	64
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	62
3			1-Hexacosene	364	C26H52	018835-33-1	62
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	62
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062542.D
Acq On : 22 Aug 2024 16:04
Operator : MA/JU
Sample : P3673-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD1

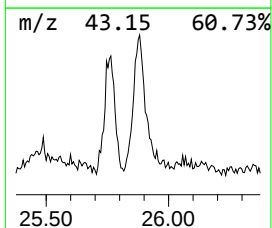
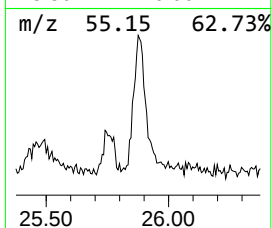
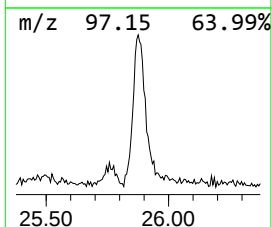
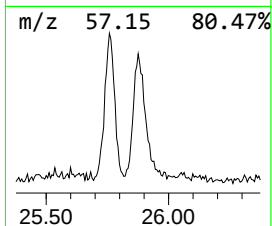
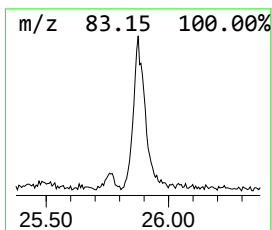
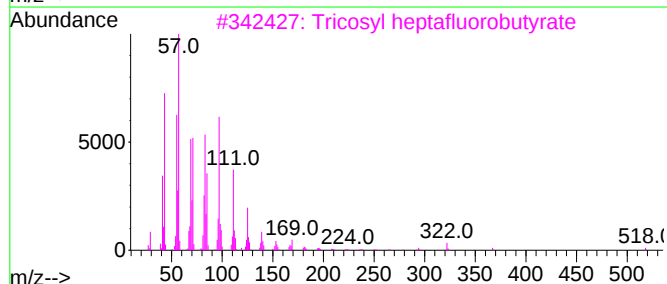
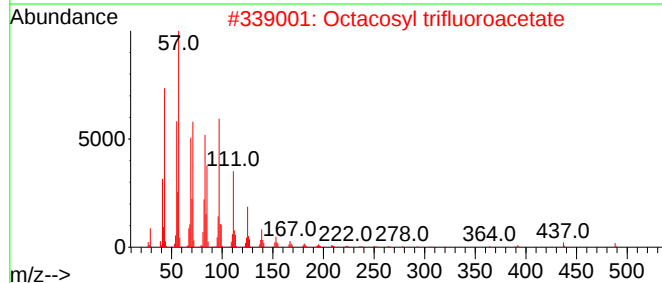
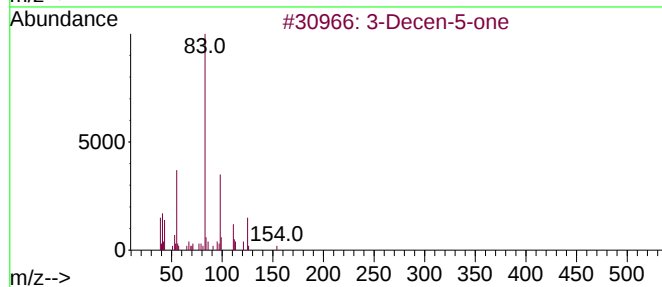
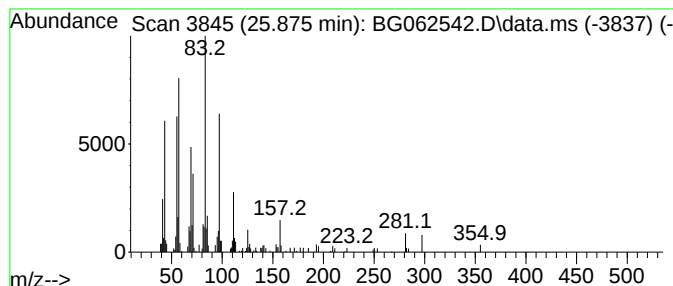
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.875	3.50 ng/ul	252579	Perylene-d12	24.636

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Decen-5-one	154	C10H18O	032064-73-6	43
2			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	38
3			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	30
4			Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	30
5			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082224\
Data File : BG062542.D
Acq On : 22 Aug 2024 16:04
Operator : MA/JU
Sample : P3673-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYD1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.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
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1-Phenoxypropan...	11.466	2.7	ng/ul	83503	2	10.731	627796	20.0
n-Hexadecanoic ...	18.198	2.4	ng/ul	168323	4	17.299	1390830	20.0
Pentadecafluoro...	21.217	2.9	ng/ul	196547	5	21.546	1367960	20.0
13-Tetradecen-1...	22.363	2.1	ng/ul	144858	5	21.546	1367960	20.0
unknown-01	25.875	3.5	ng/ul	252579	6	24.636	1443140	20.0