

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
 Data File : BG062513.D
 Acq On : 21 Aug 2024 18:05
 Operator : MA/JU
 Sample : P3626-07
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DCYF0

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: BG062513.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.403	16	19	25	rVB4	10867	17316	1.28%	0.100%
2	3.667	60	64	73	rVB	33416	53036	3.92%	0.307%
3	3.808	84	88	102	rBV	124168	204672	15.15%	1.185%
4	4.143	143	145	151	rVB3	3222	4056	0.30%	0.023%
5	4.707	240	241	244	rVB2	2701	1633	0.12%	0.009%
6	5.054	296	300	301	rBV2	2099	2570	0.19%	0.015%
7	6.029	461	466	469	rBV2	3461	4395	0.33%	0.025%
8	6.517	547	549	554	rBV3	1375	2075	0.15%	0.012%
9	6.640	565	570	573	rVB2	4593	6391	0.47%	0.037%
10	7.098	642	648	660	rVB	211328	358320	26.52%	2.075%
11	7.268	670	677	690	rVB	137857	231643	17.14%	1.342%
12	7.368	690	694	697	rBV4	933	1545	0.11%	0.009%
13	7.468	705	711	718	rBV	182969	314731	23.29%	1.823%
14	7.527	718	721	734	rVB3	6893	13433	0.99%	0.078%
15	7.938	785	791	798	rBV	228924	376296	27.85%	2.179%
16	8.003	798	802	805	rVB3	2166	2391	0.18%	0.014%
17	8.637	903	910	919	rBV	259382	442711	32.76%	2.564%
18	8.719	921	924	928	rVB2	1230	1609	0.12%	0.009%
19	9.089	980	987	999	rBV	183837	315568	23.35%	1.828%
20	9.207	1002	1007	1012	rVB4	920	1869	0.14%	0.011%
21	9.260	1012	1016	1019	rBV2	1507	2414	0.18%	0.014%
22	9.648	1076	1082	1090	rVB2	13768	21560	1.60%	0.125%
23	9.812	1100	1110	1120	rBV	148181	259350	19.19%	1.502%
24	10.352	1195	1202	1210	rBV	251604	444356	32.88%	2.573%
25	10.728	1257	1266	1274	rBV	349778	624283	46.20%	3.615%
26	10.858	1281	1288	1299	rBV	300835	542755	40.16%	3.143%
27	11.257	1353	1356	1362	rVB4	7013	10515	0.78%	0.061%
28	11.469	1386	1392	1399	rBV2	33737	64211	4.75%	0.372%
29	12.309	1529	1535	1542	rVB3	4548	6783	0.50%	0.039%
30	12.544	1571	1575	1579	rBV2	1549	2473	0.18%	0.014%
31	13.395	1715	1720	1724	rVB2	2199	3292	0.24%	0.019%
32	13.519	1738	1741	1746	rBV3	1269	1993	0.15%	0.012%
33	13.748	1778	1780	1782	rBV	1765	1717	0.13%	0.010%
34	13.965	1810	1817	1823	rBV	444912	648935	48.02%	3.758%
35	14.253	1855	1866	1877	rVV	515103	825234	61.07%	4.779%
36	14.459	1897	1901	1905	rVB5	1925	3060	0.23%	0.018%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % of largest Peak

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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

37	14.559	1911	1918	1926	rVB	632952	970332	71.81%	5.620%
38	14.664	1931	1936	1940	rVB3	921	1530	0.11%	0.009%
39	14.747	1943	1950	1963	rBV2	192138	377701	27.95%	2.187%
40	14.911	1976	1978	1981	rVB	1584	1824	0.13%	0.011%
41	14.970	1984	1988	1992	rVV3	5452	7771	0.58%	0.045%
42	15.146	2012	2018	2020	rBV2	1689	2625	0.19%	0.015%
43	15.357	2051	2054	2059	rVB4	3174	4667	0.35%	0.027%
44	15.416	2059	2064	2067	rBV3	3014	4468	0.33%	0.026%
45	15.545	2080	2086	2094	rVB	688081	1060124	78.45%	6.140%
46	15.657	2099	2105	2111	rBV	161690	232678	17.22%	1.348%
47	15.716	2113	2115	2119	rVB2	1915	1729	0.13%	0.010%
48	15.786	2123	2127	2129	rBV4	2614	3886	0.29%	0.023%
49	16.086	2176	2178	2181	rBV2	1267	1754	0.13%	0.010%
50	16.115	2181	2183	2188	rVB4	2114	2776	0.21%	0.016%
51	16.274	2207	2210	2214	rBV2	3536	3919	0.29%	0.023%
52	16.797	2293	2299	2300	rBV2	1334	2361	0.17%	0.014%
53	16.855	2304	2309	2314	rVB5	3083	5267	0.39%	0.031%
54	16.897	2314	2316	2320	rBV3	1356	2043	0.15%	0.012%
55	17.020	2333	2337	2339	rBV2	2338	2681	0.20%	0.016%
56	17.067	2341	2345	2348	rVV3	4171	5677	0.42%	0.033%
57	17.108	2348	2352	2353	rVV3	1941	2594	0.19%	0.015%
58	17.296	2377	2384	2394	rBV	780096	1169256	86.53%	6.772%
59	17.396	2394	2401	2409	rVV	791377	1154487	85.43%	6.686%
60	17.484	2412	2416	2420	rVV4	12482	16404	1.21%	0.095%
61	17.519	2420	2422	2424	rVV2	1738	1952	0.14%	0.011%
62	17.549	2425	2427	2428	rVV2	2583	1740	0.13%	0.010%
63	17.584	2430	2433	2434	rVV2	2466	2882	0.21%	0.017%
64	17.602	2434	2436	2441	rVB2	1918	3186	0.24%	0.018%
65	17.795	2467	2469	2472	rBV3	1516	2087	0.15%	0.012%
66	17.966	2495	2498	2505	rVB3	4566	7432	0.55%	0.043%
67	18.071	2510	2516	2520	rBV4	2120	3762	0.28%	0.022%
68	18.189	2531	2536	2548	rBV2	59524	105616	7.82%	0.612%
69	18.353	2562	2564	2568	rVB4	1341	1645	0.12%	0.010%
70	18.406	2571	2573	2576	rBV3	1501	1871	0.14%	0.011%
71	18.530	2590	2594	2596	rVV4	2028	2919	0.22%	0.017%
72	18.624	2607	2610	2613	rBV3	2689	2901	0.21%	0.017%
73	18.665	2615	2617	2620	rVV3	1699	1877	0.14%	0.011%
74	18.688	2620	2621	2625	rVV4	2247	2263	0.17%	0.013%
75	18.741	2628	2630	2633	rVB3	2009	1869	0.14%	0.011%
76	18.864	2647	2651	2653	rBV5	2594	3929	0.29%	0.023%

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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

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77	18.917	2659	2660	2668	rVB5	2650	3660	0.27%	0.021%
78	19.005	2672	2675	2679	rVB6	2915	4100	0.30%	0.024%
79	19.141	2696	2698	2701	rVB3	2505	2665	0.20%	0.015%
80	19.246	2711	2716	2720	rBV4	10713	16436	1.22%	0.095%
81	19.317	2724	2728	2732	rBV	15469	21580	1.60%	0.125%
82	19.464	2750	2753	2757	rBV3	12630	17310	1.28%	0.100%
83	19.564	2768	2770	2771	rVB2	2957	1639	0.12%	0.009%
84	19.575	2771	2772	2774	rBV2	2644	2360	0.17%	0.014%
85	19.616	2776	2779	2782	rVV4	8572	11536	0.85%	0.067%
86	19.681	2784	2790	2796	rVV	936427	1337576	98.98%	7.746%
87	19.728	2796	2798	2806	rVB4	19203	24834	1.84%	0.144%
88	19.887	2823	2825	2828	rBV4	3565	3953	0.29%	0.023%
89	20.122	2863	2865	2870	rBV6	2615	4196	0.31%	0.024%
90	20.198	2875	2878	2882	rVV6	4771	7210	0.53%	0.042%
91	20.486	2924	2927	2928	rBV3	3564	3597	0.27%	0.021%
92	20.609	2946	2948	2950	rVB3	3271	1698	0.13%	0.010%
93	20.656	2953	2956	2958	rVB4	8676	8324	0.62%	0.048%
94	20.709	2961	2965	2969	rBV7	6392	11353	0.84%	0.066%
95	21.208	3045	3050	3059	rBV2	89432	179700	13.30%	1.041%
96	21.537	3099	3106	3112	rBV	798250	1250752	92.56%	7.244%
97	23.764	3481	3485	3492	rVB5	17334	35081	2.60%	0.203%
98	24.404	3584	3594	3606	rVB2	492483	1300812	96.26%	7.534%
99	24.616	3619	3630	3646	rVB	479249	1351330	100.00%	7.826%
100	25.426	3753	3768	3789	rVB	104804	659550	48.81%	3.820%

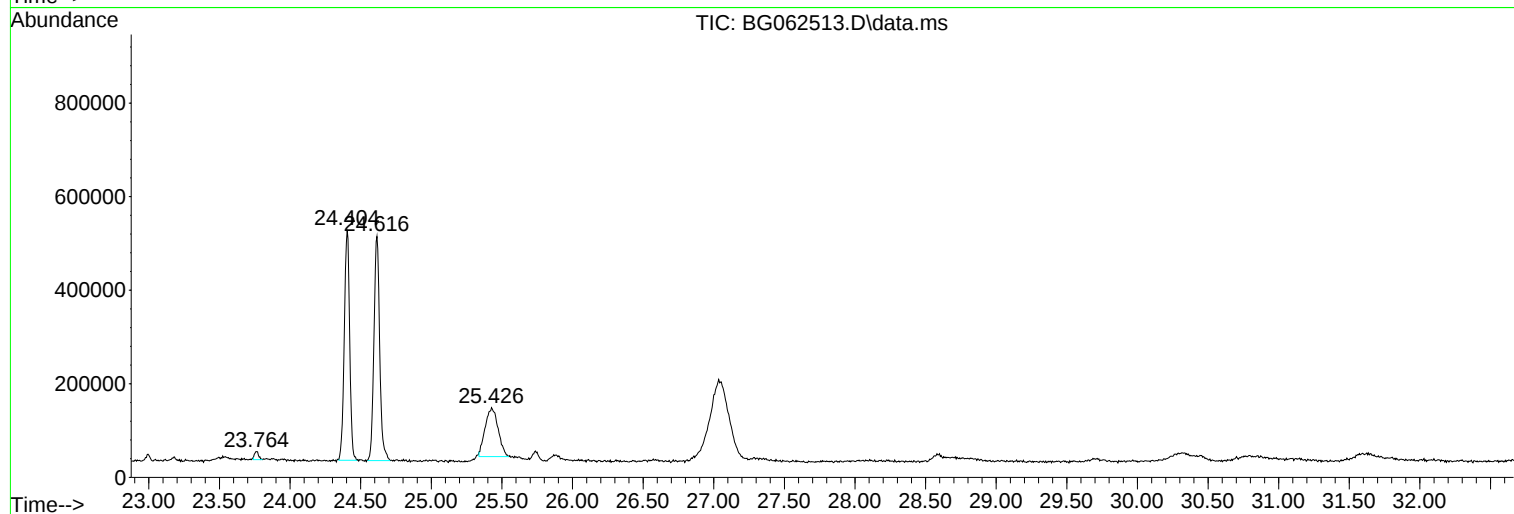
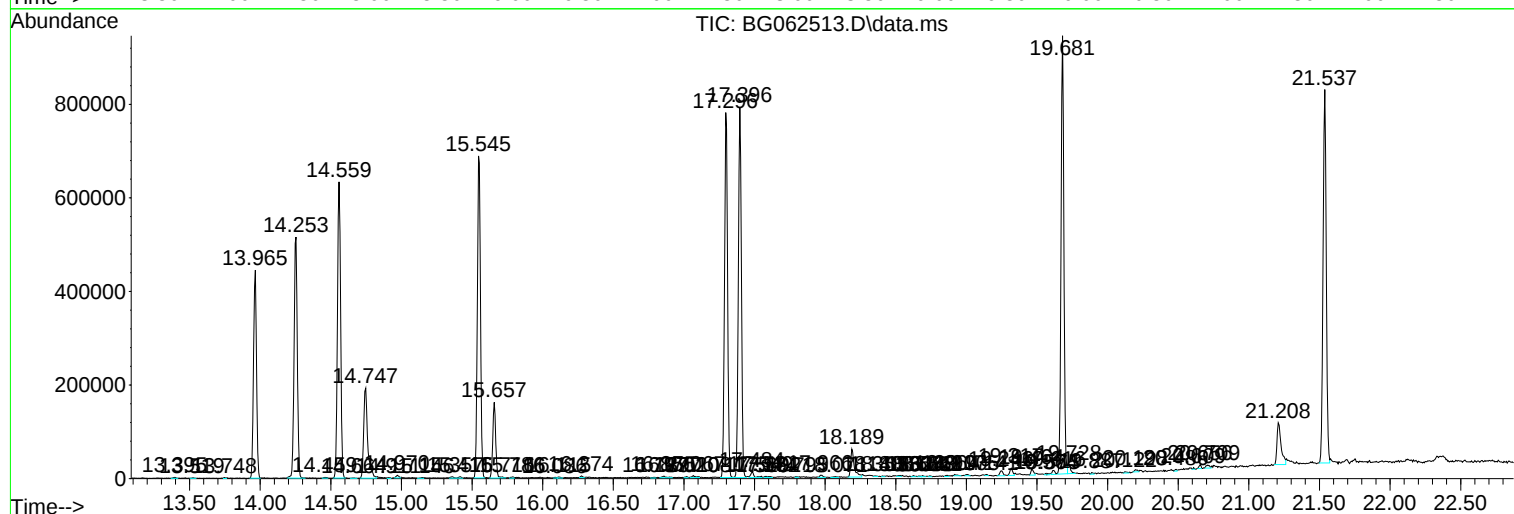
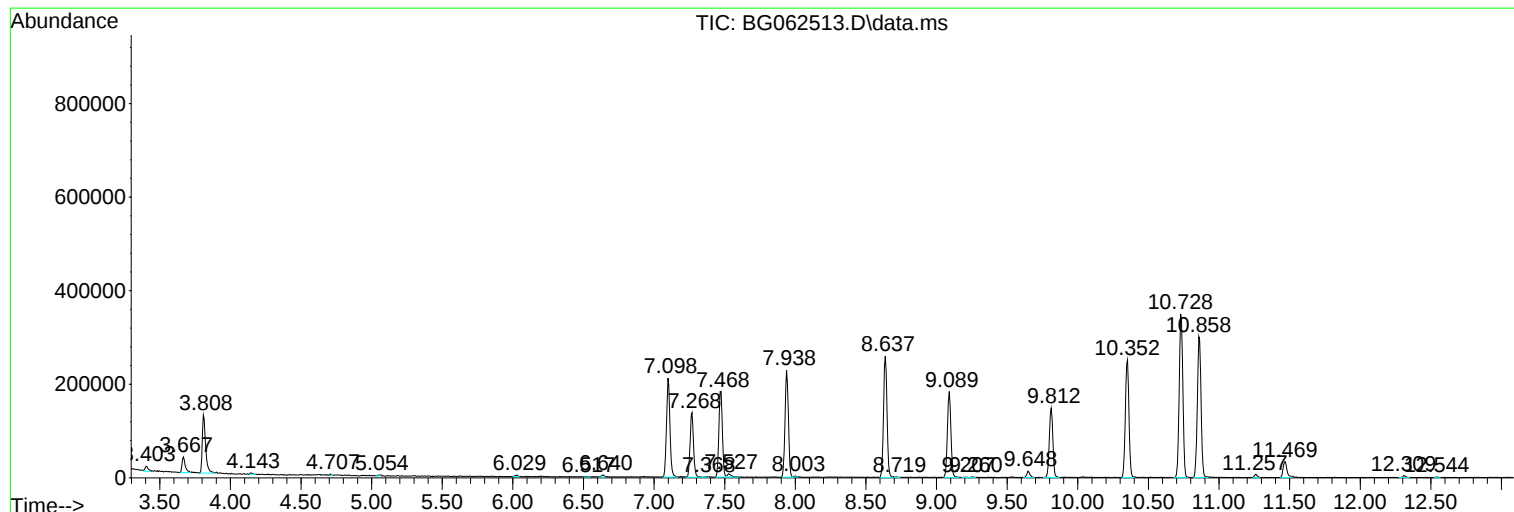
Sum of corrected areas: 17266928

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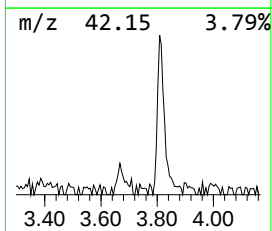
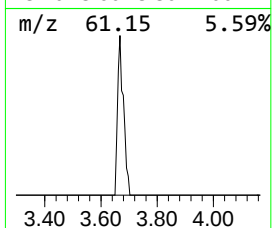
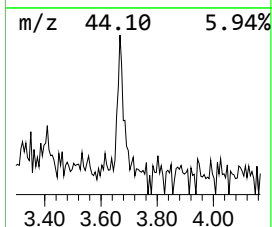
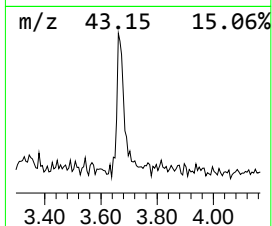
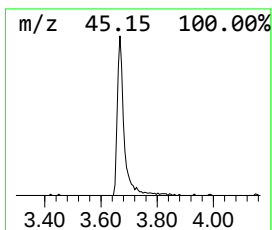
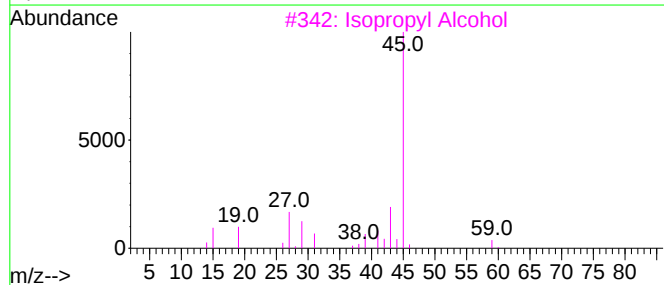
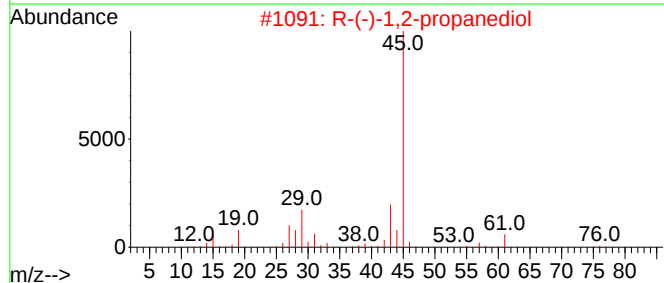
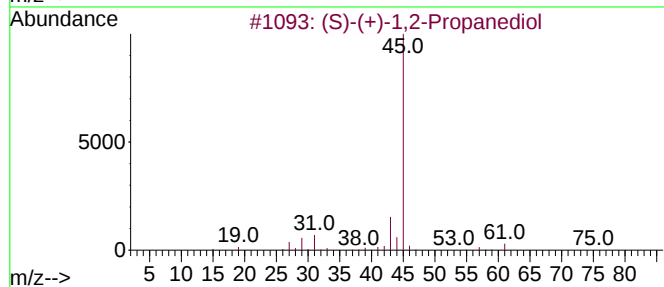
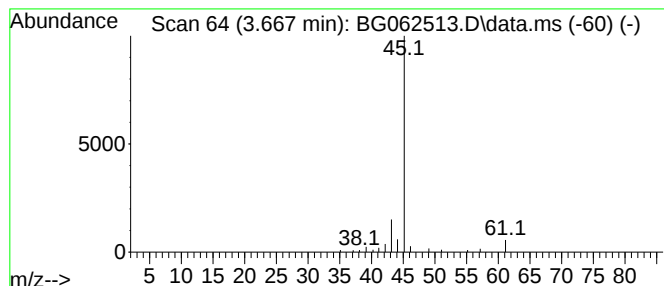
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.667	2.82 ng/ul	53036	1,4-Dichlorobenzene-d4	7.938

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	Isopropyl Alcohol			60	C3H8O	000067-63-0	9
4	Propylene Glycol			76	C3H8O2	000057-55-6	9
5	Isopropyl Alcohol			60	C3H8O	000067-63-0	9



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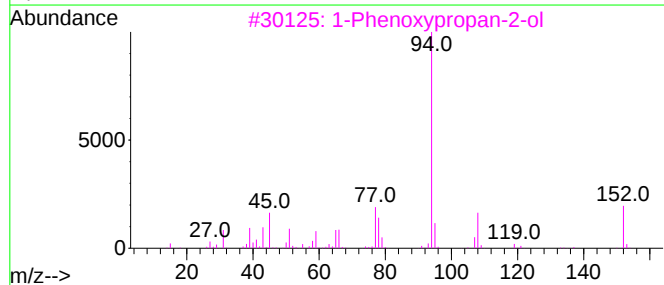
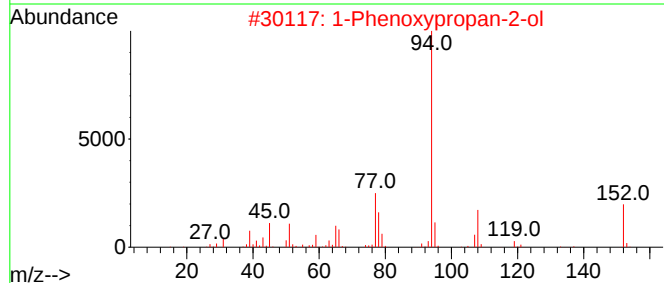
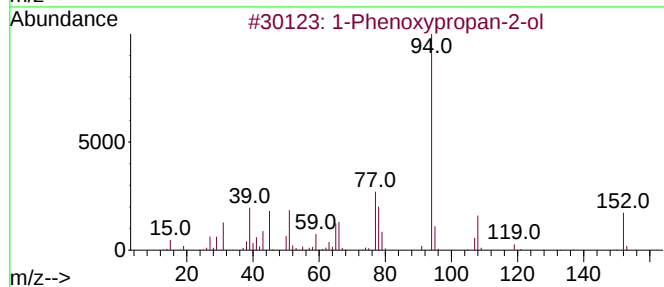
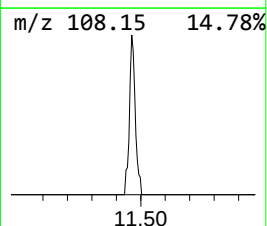
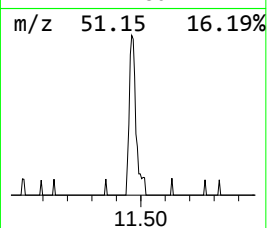
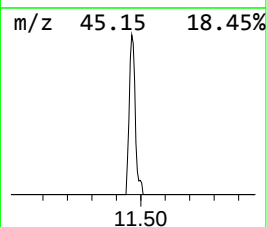
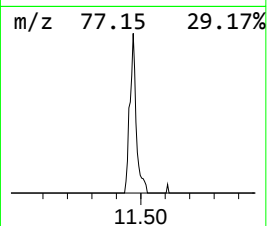
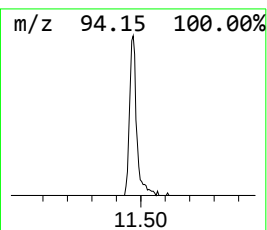
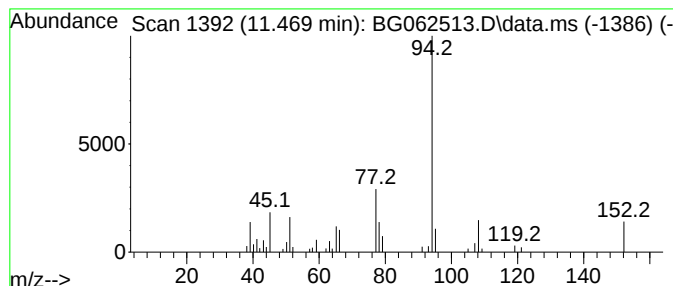
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.469	2.06 ng/ul	64211	Naphthalene-d8	10.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
3			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
4			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	81
5			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64



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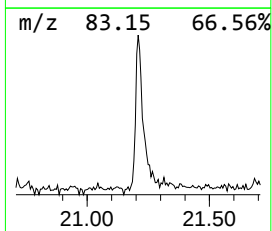
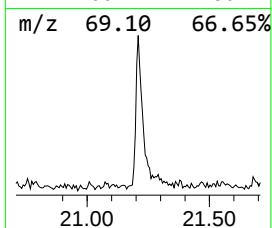
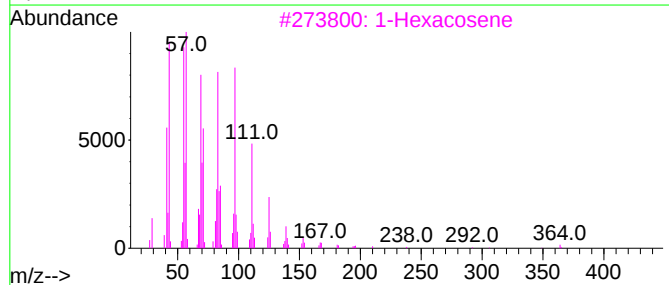
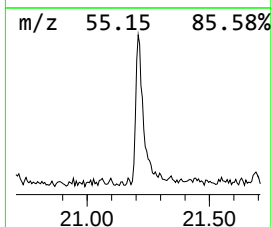
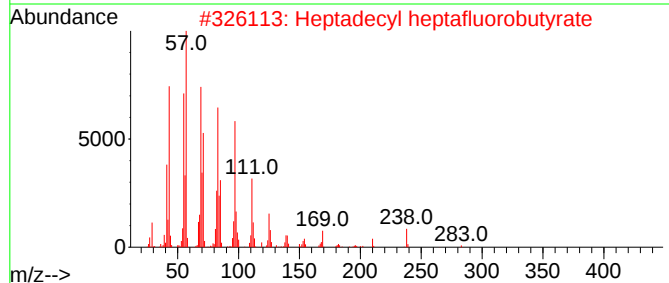
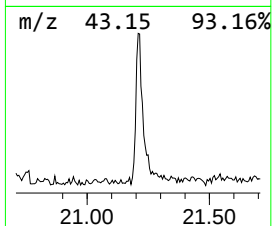
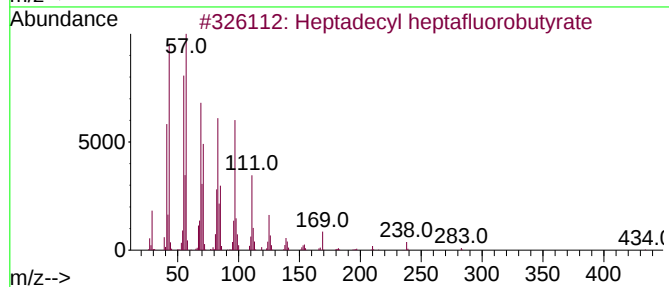
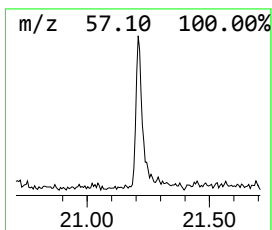
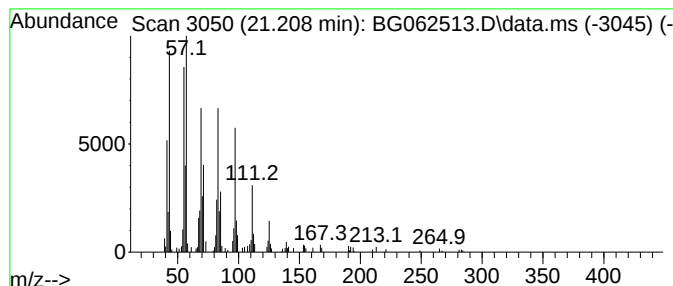
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.208	2.87 ng/ul	179700	Chrysene-d12	21.537

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3			1-Hexacosene	364	C26H52	018835-33-1	91
4			Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	91
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
Data File : BG062513.D
Acq On : 21 Aug 2024 18:05
Operator : MA/JU
Sample : P3626-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYF0

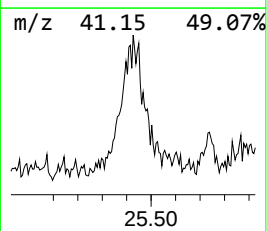
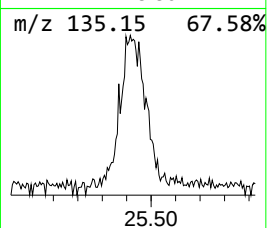
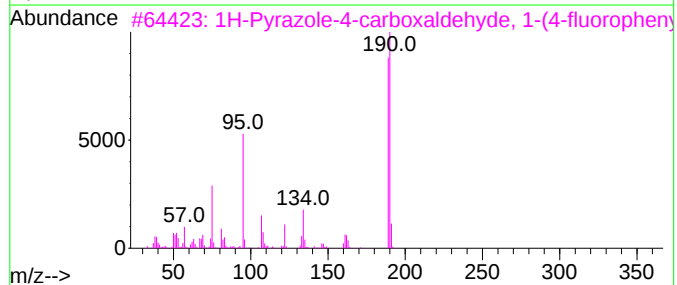
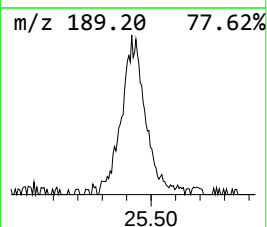
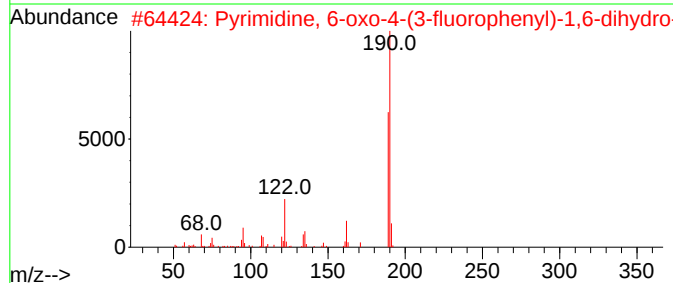
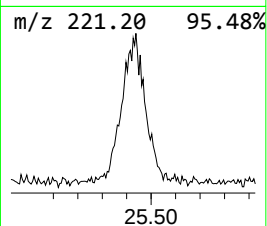
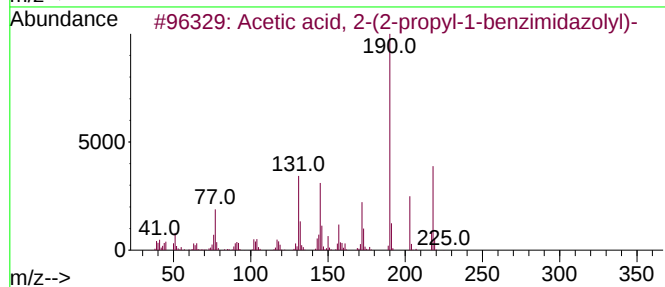
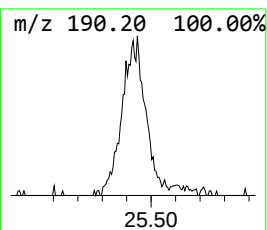
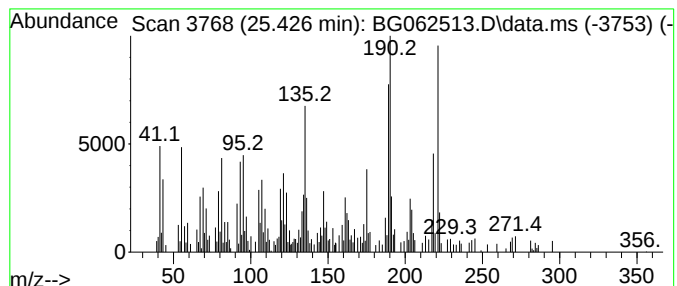
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.426	9.76 ng/ul	659550	Perylene-d12	24.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 2-(2-propyl-1-benzi...	218	C12H14N2O2	331736-92-6	43
2			Pyrimidine, 6-oxo-4-(3-fluorophe...	190	C10H7FN2O	085979-55-1	38
3			1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	38
4			6-Methoxycarbonyl-2H-1,4-benzoxa...	221	C11H11N04	861348-36-9	38
5			6-Fluoro-4-hydroxy-N-(pyrimidin-...	284	C14H9FN4O2	1000409-44-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082124\
Data File : BG062513.D
Acq On : 21 Aug 2024 18:05
Operator : MA/JU
Sample : P3626-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYF0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(S)-(+)-1,2-Pro...	3.667	2.8	ng/ul	53036	1	7.938	376296	20.0
1-Phenoxypropan...	11.469	2.1	ng/ul	64211	2	10.728	624283	20.0
Heptadecyl hept...	21.208	2.9	ng/ul	179700	5	21.537	1250750	20.0
unknown-01	25.426	9.8	ng/ul	659550	6	24.616	1351330	20.0