

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
 Data File : BG062348.D
 Acq On : 9 Aug 2024 5:13
 Operator : MA/JU
 Sample : P3434-06
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 E05T7

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: BG062348.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.419	19	22	26	rBV4	8037	11056	0.74%	0.059%
2	3.684	63	67	75	rBV	23962	40960	2.75%	0.217%
3	3.825	86	91	106	rBV	122846	211623	14.21%	1.124%
4	4.159	146	148	154	rVB3	3717	5875	0.39%	0.031%
5	6.039	463	468	474	rBV3	7882	13566	0.91%	0.072%
6	6.656	568	573	579	rBV3	14607	22110	1.48%	0.117%
7	6.938	616	621	625	rBV2	3787	5804	0.39%	0.031%
8	7.108	642	650	660	rBV	180316	328272	22.05%	1.743%
9	7.285	674	680	693	rBV	130802	219585	14.75%	1.166%
10	7.490	707	715	721	rBV	168580	292292	19.63%	1.552%
11	7.549	721	725	731	rVB2	8759	13737	0.92%	0.073%
12	7.954	787	794	802	rBV	206187	365030	24.51%	1.938%
13	8.019	802	805	810	rVB3	5136	8077	0.54%	0.043%
14	8.648	905	912	922	rBV	220210	388305	26.08%	2.062%
15	9.106	983	990	999	rBV	170998	301141	20.22%	1.599%
16	9.670	1079	1086	1093	rBV2	27390	43133	2.90%	0.229%
17	9.828	1106	1113	1123	rBV	146388	255866	17.18%	1.359%
18	10.239	1177	1183	1189	rBV3	6031	10809	0.73%	0.057%
19	10.363	1197	1204	1212	rBV	251539	438357	29.44%	2.328%
20	10.751	1262	1270	1277	rVV	349979	611686	41.08%	3.248%
21	10.874	1283	1291	1303	rVB	233617	417762	28.06%	2.218%
22	11.279	1354	1360	1364	rBV4	9576	14405	0.97%	0.076%
23	11.485	1388	1395	1402	rBV2	46970	83335	5.60%	0.442%
24	12.231	1517	1522	1525	rVV3	4085	6293	0.42%	0.033%
25	12.331	1533	1539	1544	rBV	4393	7449	0.50%	0.040%
26	12.407	1546	1552	1557	rBV4	3180	6090	0.41%	0.032%
27	13.412	1719	1723	1728	rBV2	5059	6948	0.47%	0.037%
28	13.981	1812	1820	1826	rVV	459712	671496	45.10%	3.565%
29	14.269	1855	1869	1879	rBV	522786	863851	58.01%	4.587%
30	14.434	1893	1897	1901	rVB4	5742	6397	0.43%	0.034%
31	14.575	1912	1921	1929	rBV	586390	918213	61.67%	4.875%
32	14.751	1945	1951	1958	rBV	190046	360988	24.24%	1.917%
33	14.827	1963	1964	1968	rVB3	6582	6374	0.43%	0.034%
34	14.980	1985	1990	1995	rBV4	4248	7770	0.52%	0.041%
35	15.380	2053	2058	2063	rVV4	5716	8883	0.60%	0.047%
36	15.562	2082	2089	2101	rBV	708312	1087806	73.05%	5.776%

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Integrator: RTE

Smoothing : OFF

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
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37	15.667	2101	2107	2116	rBV	145428	218566	14.68%	1.161%
38	15.744	2116	2120	2124	rVB4	11982	17144	1.15%	0.091%
39	16.120	2180	2184	2187	rBV3	7006	10581	0.71%	0.056%
40	16.296	2209	2214	2217	rBV2	6873	10008	0.67%	0.053%
41	16.825	2297	2304	2309	rBV7	4391	8499	0.57%	0.045%
42	16.883	2309	2314	2319	rBV6	7770	14787	0.99%	0.079%
43	17.089	2345	2349	2352	rBV3	4698	7008	0.47%	0.037%
44	17.130	2352	2356	2362	rVB5	6323	12707	0.85%	0.067%
45	17.212	2366	2370	2373	rBV3	12308	15139	1.02%	0.080%
46	17.312	2378	2387	2393	rVV	719101	1084055	72.80%	5.756%
47	17.353	2393	2394	2398	rVV	19594	16150	1.08%	0.086%
48	17.412	2398	2404	2411	rVV	711269	1084873	72.86%	5.760%
49	17.494	2414	2418	2421	rVB5	6171	9533	0.64%	0.051%
50	17.559	2424	2429	2433	rBV4	12381	19080	1.28%	0.101%
51	17.659	2442	2446	2450	rVB3	16092	21471	1.44%	0.114%
52	17.906	2483	2488	2493	rBV3	11256	17739	1.19%	0.094%
53	17.988	2498	2502	2507	rVB7	10305	18129	1.22%	0.096%
54	18.094	2514	2520	2525	rBV3	20011	39034	2.62%	0.207%
55	18.152	2525	2530	2535	rVV	68759	102320	6.87%	0.543%
56	18.211	2535	2540	2551	rVB	242408	370103	24.86%	1.965%
57	18.517	2586	2592	2597	rBV7	12271	24878	1.67%	0.132%
58	18.681	2617	2620	2624	rBV6	5884	6702	0.45%	0.036%
59	18.757	2629	2633	2636	rBV5	7004	9642	0.65%	0.051%
60	18.881	2650	2654	2658	rVB6	4197	7699	0.52%	0.041%
61	19.092	2685	2690	2694	rVV7	16130	26014	1.75%	0.138%
62	19.163	2696	2702	2710	rVB8	11314	23764	1.60%	0.126%
63	19.257	2714	2718	2722	rVB4	12190	15351	1.03%	0.082%
64	19.339	2727	2732	2733	rBV3	32269	46303	3.11%	0.246%
65	19.362	2733	2736	2748	rVB2	77981	139520	9.37%	0.741%
66	19.480	2752	2756	2763	rBV	67749	96236	6.46%	0.511%
67	19.633	2780	2782	2786	rVB4	8534	9513	0.64%	0.051%
68	19.691	2786	2792	2800	rBV	970989	1426745	95.82%	7.576%
69	19.750	2800	2802	2806	rVB	24775	29907	2.01%	0.159%
70	19.856	2816	2820	2823	rBV4	8899	10824	0.73%	0.057%
71	20.208	2877	2880	2884	rBV4	12136	18103	1.22%	0.096%
72	20.249	2885	2887	2893	rVV5	8025	9673	0.65%	0.051%
73	20.308	2895	2897	2902	rVB6	4518	6657	0.45%	0.035%
74	20.373	2904	2908	2910	rVB5	5585	8571	0.58%	0.046%
75	20.590	2943	2945	2948	rVB4	5411	5844	0.39%	0.031%
76	20.678	2958	2960	2962	rVB3	8874	6327	0.42%	0.034%

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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 >
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 Title : SVOA CALIBRATION

77	20.719	2964	2967	2968	rBV3	7075	6565	0.44%	0.035%
78	20.772	2973	2976	2980	rVB3	15286	18224	1.22%	0.097%
79	21.131	3033	3037	3038	rBV4	7961	8917	0.60%	0.047%
80	21.195	3043	3048	3049	rBV5	12017	15597	1.05%	0.083%
81	21.225	3049	3053	3060	rVV	118750	175925	11.81%	0.934%
82	21.548	3100	3108	3114	rBV2	750891	1278178	85.84%	6.787%
83	21.771	3143	3146	3152	rVB2	16568	23169	1.56%	0.123%
84	22.006	3182	3186	3191	rVB7	15140	22641	1.52%	0.120%
85	22.370	3244	3248	3257	rVB4	38382	79702	5.35%	0.423%
86	23.040	3358	3362	3366	rVB3	20746	30417	2.04%	0.162%
87	23.662	3462	3468	3473	rBV5	17732	42474	2.85%	0.226%
88	23.815	3488	3494	3500	rBV	35851	68654	4.61%	0.365%
89	24.426	3588	3598	3615	rVB	550841	1489034	100.00%	7.906%
90	24.638	3623	3634	3645	rBV	482480	1326434	89.08%	7.043%
91	24.726	3645	3649	3661	rVB6	24106	62840	4.22%	0.334%
92	25.818	3827	3835	3845	rBV3	28321	83687	5.62%	0.444%
93	26.758	3991	3995	3996	rBV4	8740	10335	0.69%	0.055%
94	27.117	4048	4056	4057	rBV4	16134	31114	2.09%	0.165%
95	28.679	4312	4322	4323	rBV6	127344	256652	17.24%	1.363%
96	29.126	4386	4398	4410	rBV9	73548	325436	21.86%	1.728%
97	29.754	4493	4505	4519	rBV9	43279	225162	15.12%	1.196%
98	31.152	4732	4743	4744	rBV10	32192	75452	5.07%	0.401%
99	31.522	4803	4806	4807	rBV3	6336	6480	0.44%	0.034%
100	31.775	4840	4849	4851	rBV7	32545	83700	5.62%	0.444%

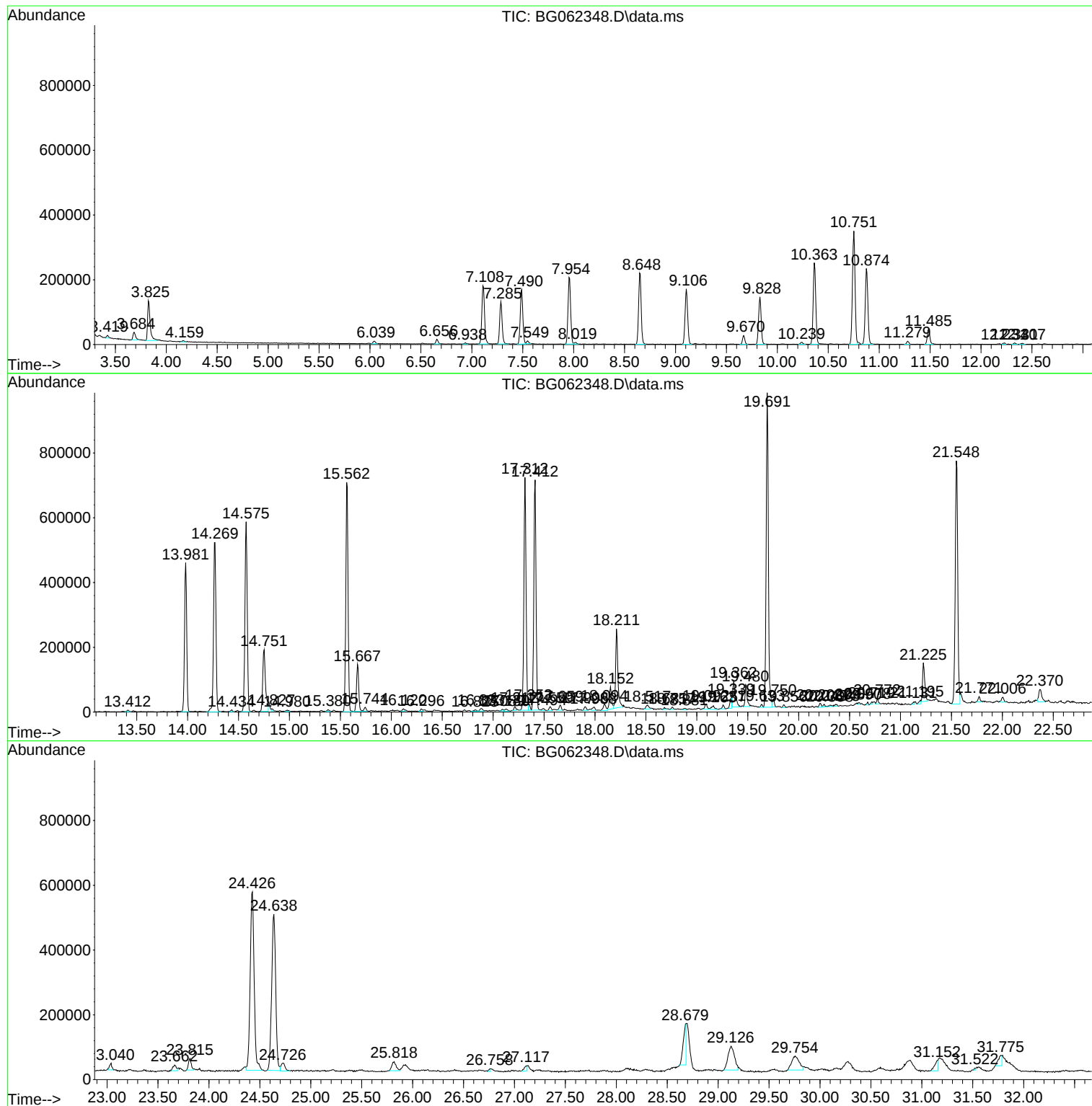
Sum of corrected areas: 18833332

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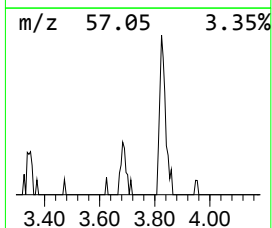
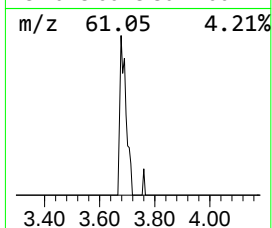
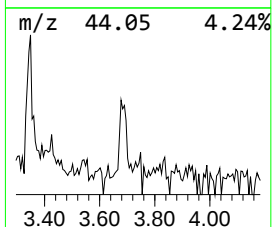
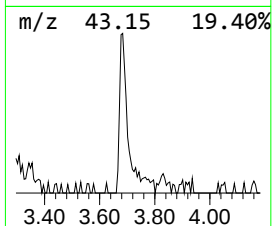
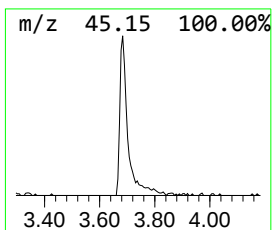
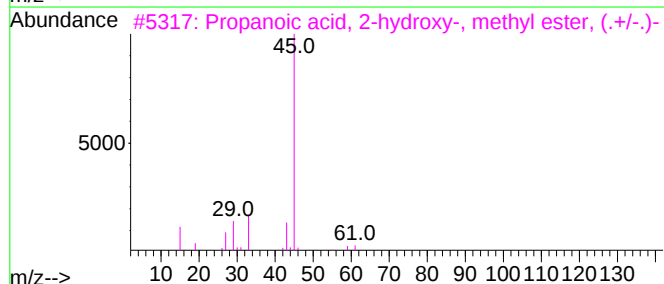
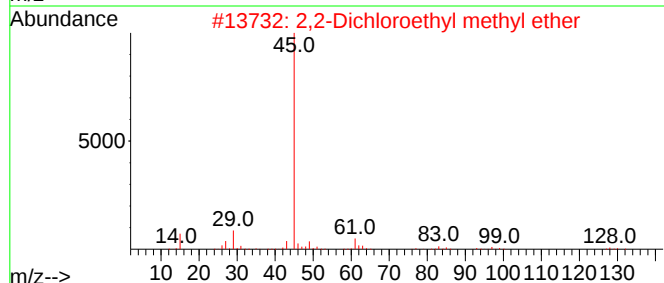
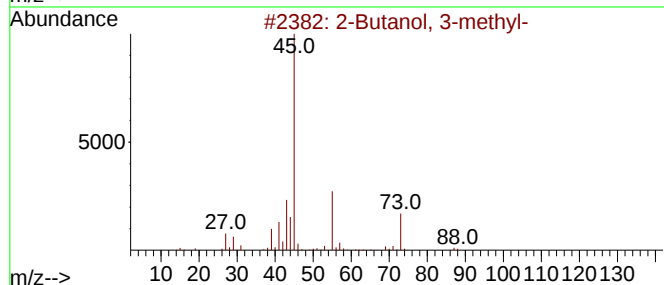
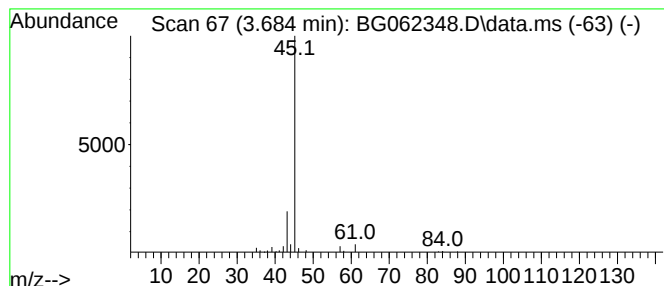
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.684	2.24 ng/ul	40960	1,4-Dichlorobenzene-d4	7.960

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 3-methyl-			88	C5H12O	000598-75-4	9
2	2,2-Dichloroethyl methyl ether			128	C3H6Cl2O	034862-07-2	9
3	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	9
4	Propylene Glycol			76	C3H8O2	000057-55-6	9
5	Isopropyl Alcohol			60	C3H8O	000067-63-0	9



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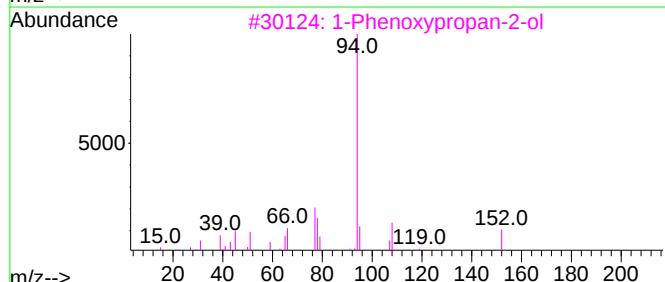
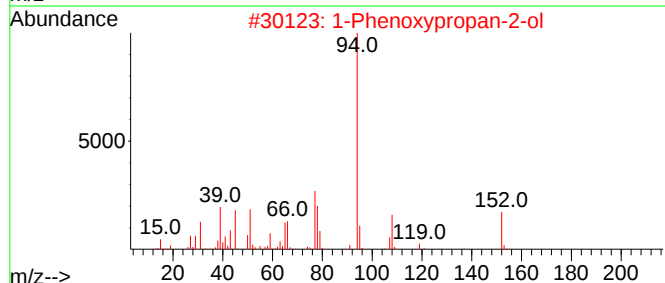
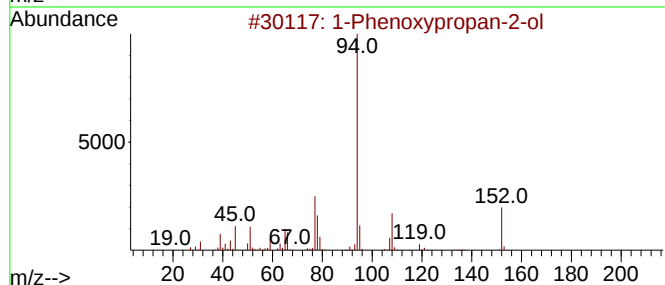
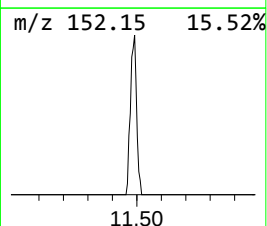
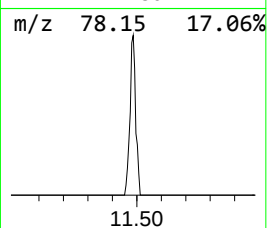
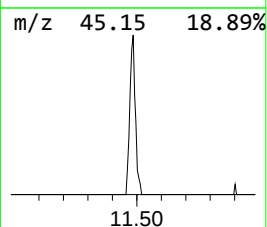
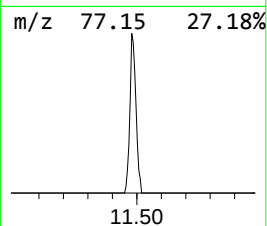
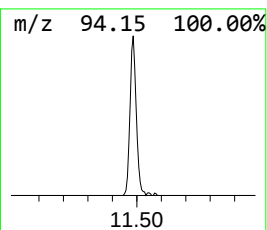
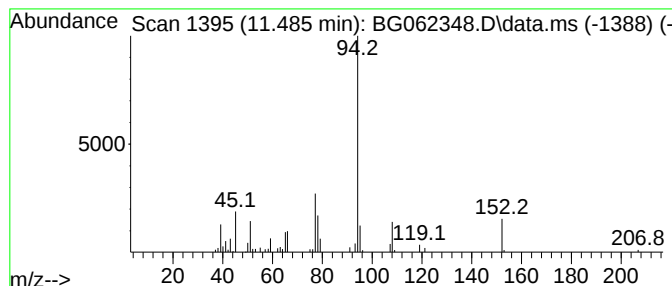
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.485	2.72 ng/ul	83335	Naphthalene-d8	10.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
3			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	83
4			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	80
5			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64



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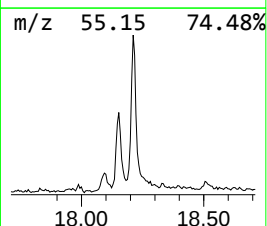
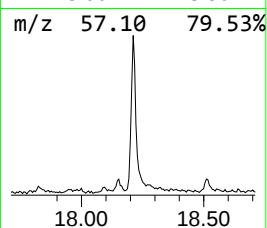
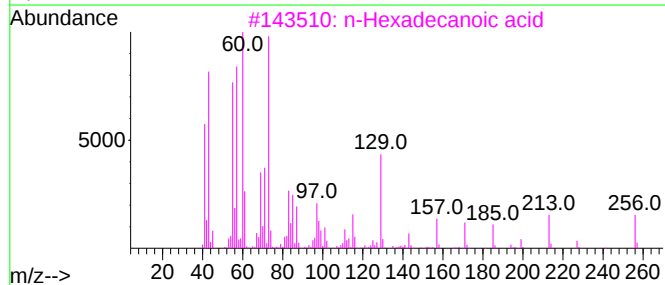
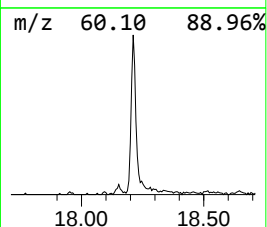
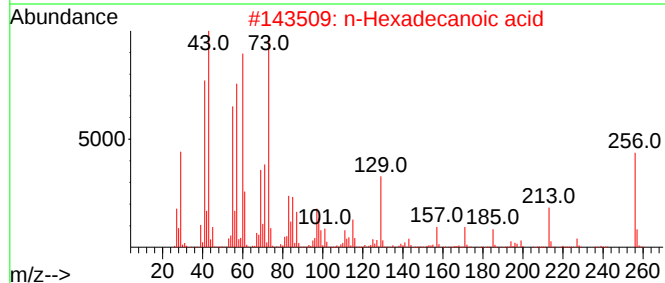
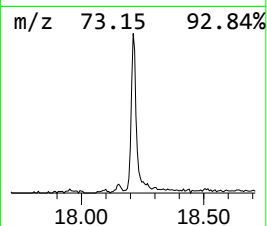
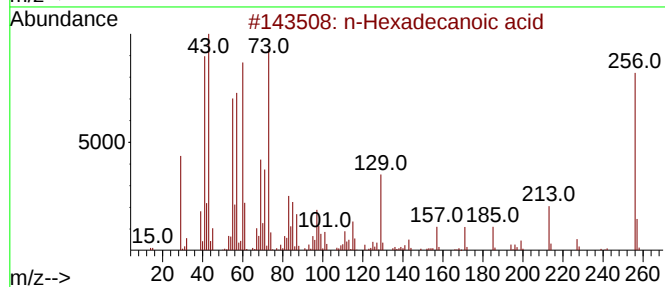
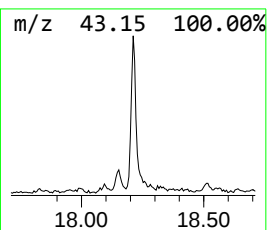
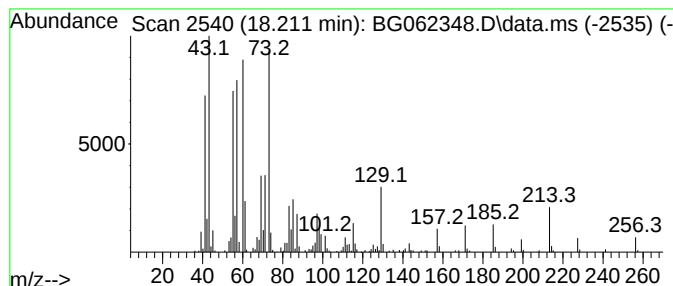
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	6.83 ng/ul	370103	Phenanthrene-d10	17.312

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062348.D
Acq On : 9 Aug 2024 5:13
Operator : MA/JU
Sample : P3434-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05T7

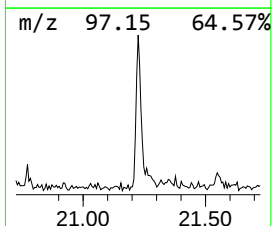
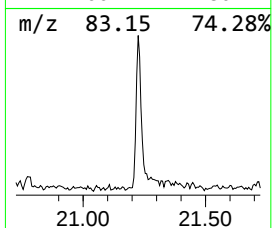
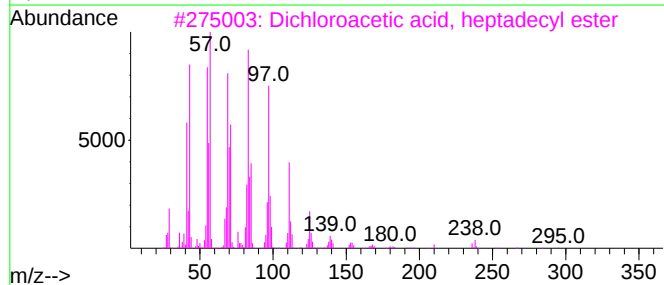
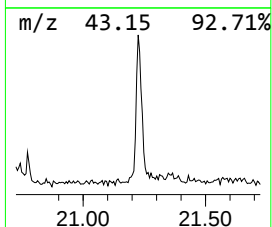
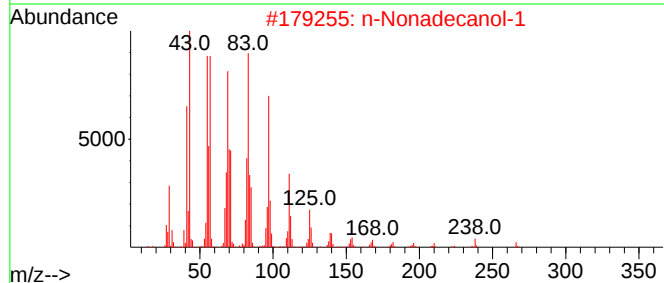
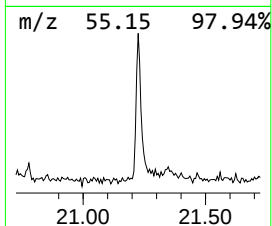
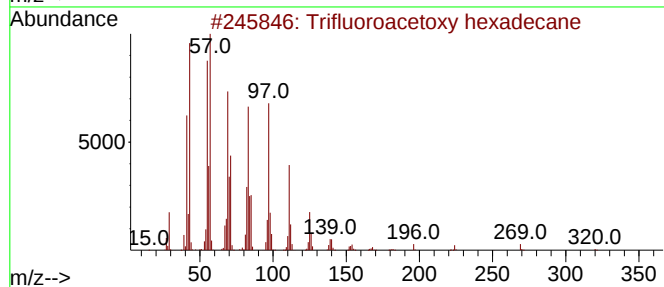
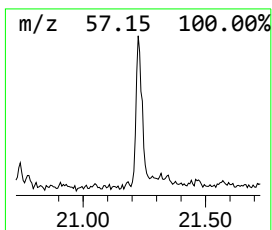
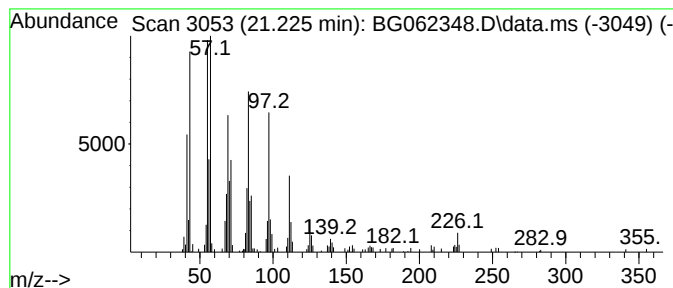
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.225	2.75 ng/ul	175925	Chrysene-d12	21.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062348.D
Acq On : 9 Aug 2024 5:13
Operator : MA/JU
Sample : P3434-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05T7

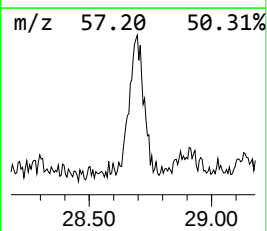
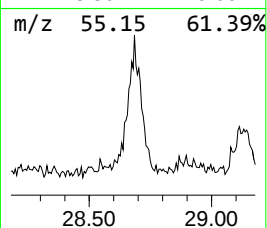
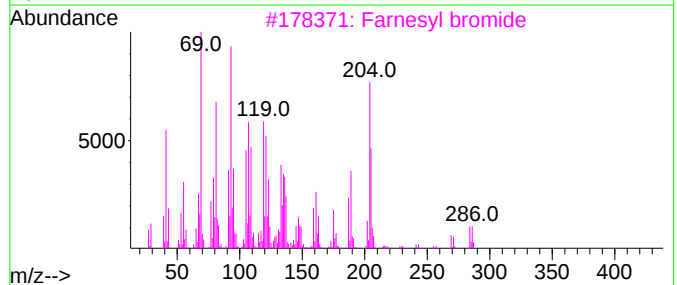
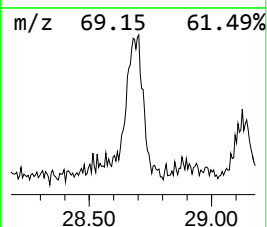
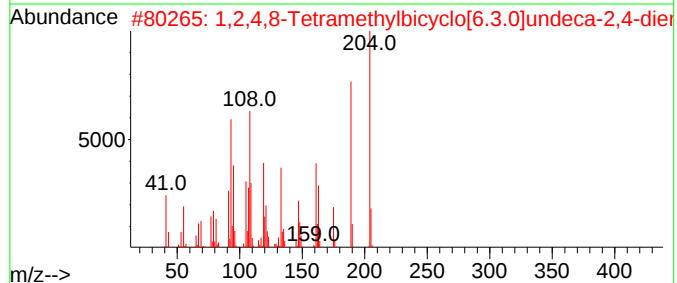
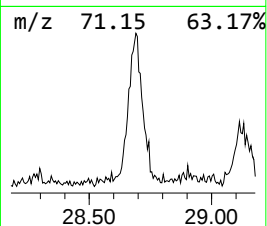
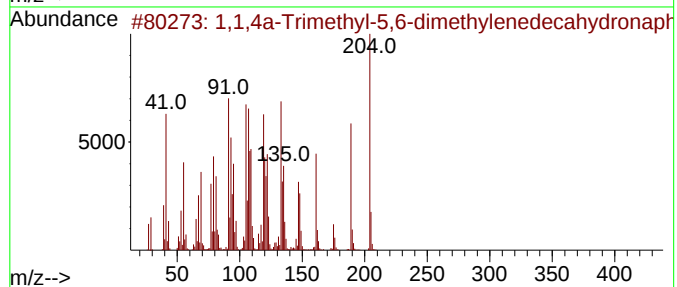
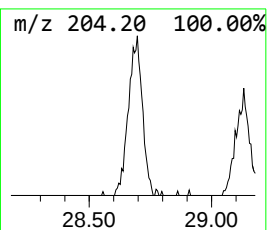
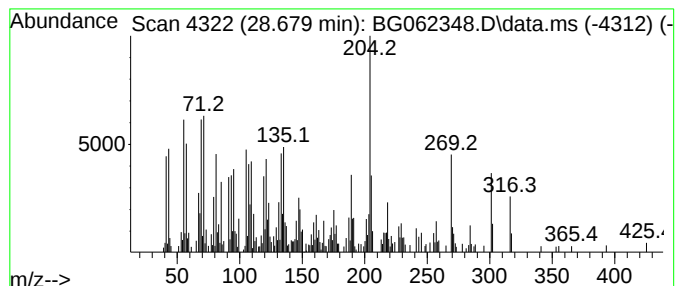
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.679	3.87 ng/ul	256652	Perylene-d12	24.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	58		
2	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	52		
3	Farnesyl bromide	284	C15H25Br	006874-67-5	50		
4	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	49		
5	Labda-7,14-dien-13(R)-ol	290	C20H34O	1010428-65-8	46		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062348.D
Acq On : 9 Aug 2024 5:13
Operator : MA/JU
Sample : P3434-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05T7

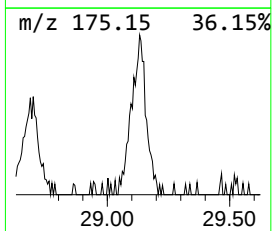
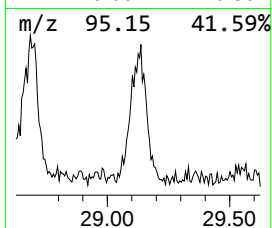
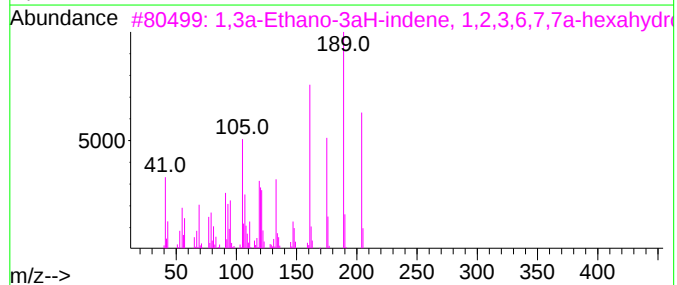
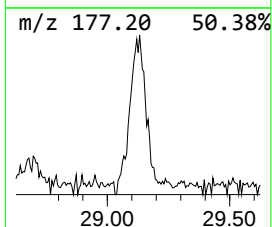
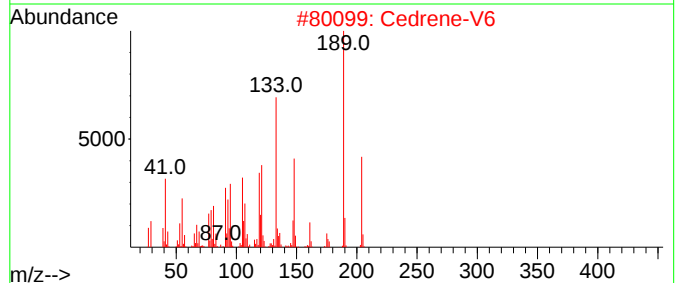
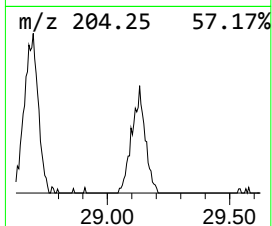
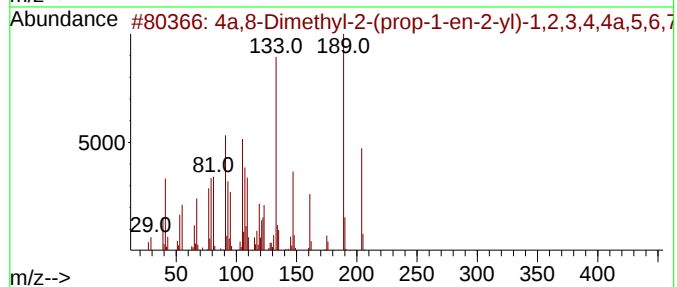
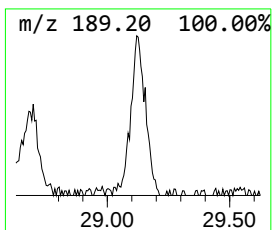
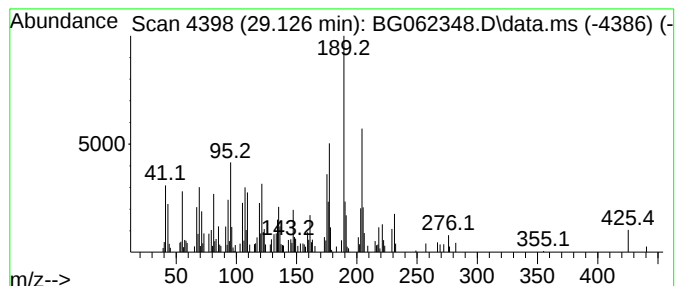
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 4a,8-Dimethyl-2-(prop-1-en-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.126	4.91 ng/ul	325436	Perylene-d12	24.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	55
2			Cedrene-V6	204	C15H24	1000162-76-8	49
3			1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	46
4			3,4-Dihydrocoumarin, 4,4-dimethy...	204	C13H16O2	029423-74-3	42
5			2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	001209-71-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062348.D
Acq On : 9 Aug 2024 5:13
Operator : MA/JU
Sample : P3434-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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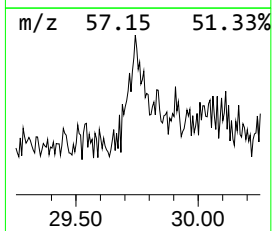
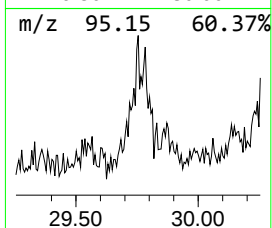
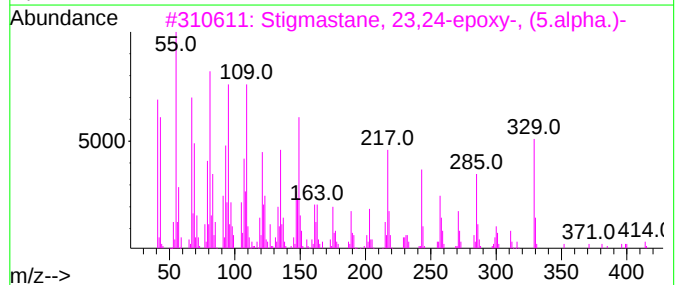
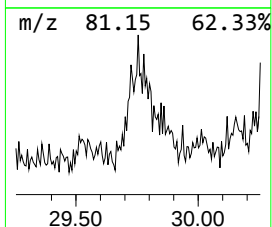
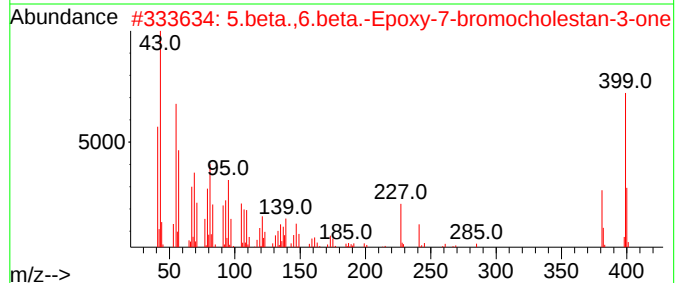
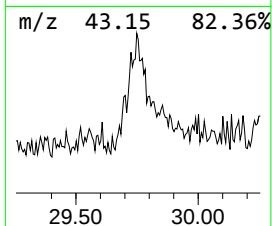
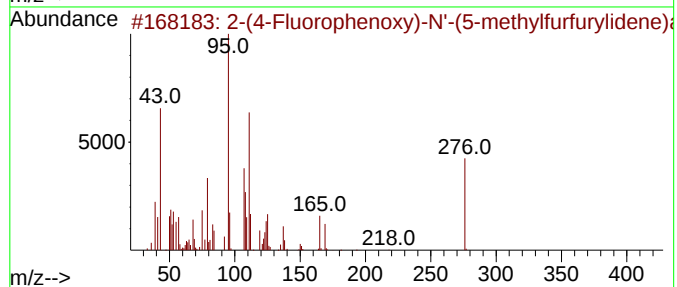
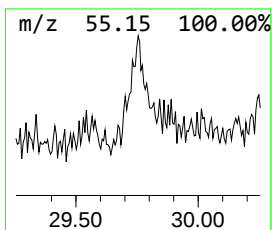
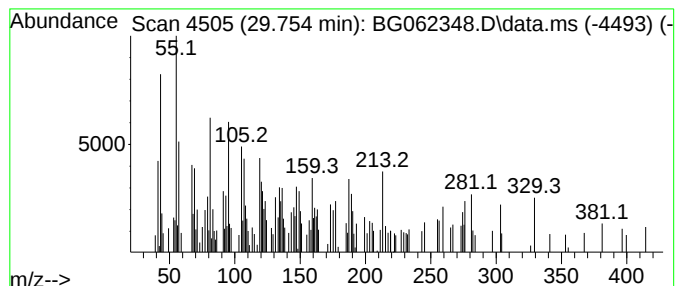
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.754	3.40 ng/ul	225162	Perylene-d12	24.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Fluorophenoxy)-N'-(5-methyl...	276	C14H13FN2O3	339121-32-3	38		
2	5.beta.,6.beta.-Epoxy-7-bromocho...	478	C27H43BrO2	104825-82-3	27		
3	Stigmastane, 23,24-epoxy-, (5.alpha...	414	C29H50O	054411-91-5	25		
4	2H-Cyclohepta[b]furan-2-one, 3,3...	248	C15H20O3	033649-15-9	16		
5	1,1,4,7-Tetramethyldecahydro-1H...	238	C15H26O2	121221-43-2	16		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062348.D
Acq On : 9 Aug 2024 5:13
Operator : MA/JU
Sample : P3434-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05T7

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
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1-Phenoxypropan...	11.485	2.7	ng/ul	83335	2	10.751	611686	20.0
n-Hexadecanoic ...	18.211	6.8	ng/ul	370103	4	17.312	1084060	20.0
Trifluoroacetox...	21.225	2.8	ng/ul	175925	5	21.548	1278180	20.0
1,1,4a-Trimethy...	28.679	3.9	ng/ul	256652	6	24.638	1326430	20.0
4a,8-Dimethyl-2...	29.126	4.9	ng/ul	325436	6	24.638	1326430	20.0
unknown-02	29.754	3.4	ng/ul	225162	6	24.638	1326430	20.0