

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
 Data File : BG062346.D
 Acq On : 9 Aug 2024 3:51
 Operator : MA/JU
 Sample : P3434-04
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 E05T5

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: BG062346.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.341	7	9	16	rVB4	5775	8717	0.31%	0.035%
2	3.423	19	23	30	rVB2	10546	19157	0.69%	0.076%
3	3.681	63	67	76	rVB	16388	27424	0.99%	0.109%
4	3.822	87	91	106	rVB	116691	199006	7.17%	0.792%
5	6.043	465	469	474	rVB2	9218	13230	0.48%	0.053%
6	7.112	643	651	663	rVB	248406	433072	15.60%	1.724%
7	7.282	674	680	690	rBV	165633	282933	10.19%	1.127%
8	7.488	708	715	722	rBV	221213	374496	13.49%	1.491%
9	7.547	722	725	731	rVV3	6938	9965	0.36%	0.040%
10	7.958	788	795	802	rBV	210300	355802	12.82%	1.417%
11	8.017	802	805	810	rVB2	7356	9766	0.35%	0.039%
12	8.651	904	913	922	rBV	316339	535218	19.28%	2.131%
13	9.109	980	991	1000	rBV	225338	401741	14.47%	1.600%
14	9.667	1079	1086	1094	rBV2	31446	49662	1.79%	0.198%
15	9.826	1106	1113	1126	rBV	183660	330295	11.90%	1.315%
16	10.237	1177	1183	1189	rBV5	4797	9718	0.35%	0.039%
17	10.366	1195	1205	1215	rBV	333424	588840	21.21%	2.345%
18	10.748	1259	1270	1278	rBV	339875	600685	21.64%	2.392%
19	10.877	1284	1292	1304	rBV	310816	552165	19.89%	2.199%
20	11.283	1355	1361	1367	rBV2	14158	22203	0.80%	0.088%
21	11.482	1387	1395	1402	rBV2	69030	128385	4.62%	0.511%
22	12.228	1517	1522	1528	rVB2	4273	6598	0.24%	0.026%
23	12.334	1534	1540	1544	rVB2	6470	10798	0.39%	0.043%
24	13.415	1720	1724	1729	rVB3	6092	7888	0.28%	0.031%
25	13.979	1810	1820	1827	rBV	606847	895991	32.28%	3.567%
26	14.073	1829	1836	1839	rVV4	3710	6266	0.23%	0.025%
27	14.226	1856	1862	1863	rBV	13850	17947	0.65%	0.071%
28	14.267	1863	1869	1877	rVV	725105	1124908	40.52%	4.479%
29	14.484	1902	1906	1911	rBV2	5662	7835	0.28%	0.031%
30	14.572	1915	1921	1928	rVV	599061	914008	32.92%	3.639%
31	14.749	1943	1951	1955	rBV	212447	358458	12.91%	1.427%
32	14.984	1986	1991	1995	rBV7	3958	7799	0.28%	0.031%
33	15.377	2053	2058	2064	rVV5	6758	13036	0.47%	0.052%
34	15.436	2064	2068	2072	rVV	8036	9896	0.36%	0.039%
35	15.565	2082	2090	2102	rVB	953540	1427097	51.41%	5.682%
36	15.671	2102	2108	2117	rBV	177197	270376	9.74%	1.077%

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37	15.841	2134	2137	2142	rVB2	4554	6308	0.23%	0.025%
38	16.117	2180	2184	2192	rVB4	7192	13323	0.48%	0.053%
39	16.299	2210	2215	2217	rBV2	10772	15432	0.56%	0.061%
40	16.323	2217	2219	2229	rVB5	12014	16688	0.60%	0.066%
41	16.875	2307	2313	2317	rBV6	5465	9129	0.33%	0.036%
42	17.087	2344	2349	2354	rVV6	10430	16296	0.59%	0.065%
43	17.134	2354	2357	2363	rVB4	5168	9502	0.34%	0.038%
44	17.210	2363	2370	2374	rBV5	11523	23794	0.86%	0.095%
45	17.310	2378	2387	2393	rVV	735772	1092381	39.35%	4.349%
46	17.351	2393	2394	2398	rVV	18283	17104	0.62%	0.068%
47	17.410	2398	2404	2411	rVV	953090	1440083	51.87%	5.734%
48	17.492	2414	2418	2424	rBV8	5659	11782	0.42%	0.047%
49	17.598	2433	2436	2439	rBV5	5273	6369	0.23%	0.025%
50	17.703	2449	2454	2459	rVB5	4885	7099	0.26%	0.028%
51	17.827	2472	2475	2477	rBV2	6742	7443	0.27%	0.030%
52	17.980	2494	2501	2510	rVB2	74689	121943	4.39%	0.486%
53	18.091	2514	2520	2525	rBV4	19096	36498	1.31%	0.145%
54	18.150	2525	2530	2536	rBV2	53178	80102	2.89%	0.319%
55	18.215	2536	2541	2552	rVV	304121	440024	15.85%	1.752%
56	18.514	2588	2592	2597	rBV5	19574	30831	1.11%	0.123%
57	18.643	2610	2614	2617	rVV5	7152	8467	0.30%	0.034%
58	18.684	2617	2621	2630	rVV6	9386	21396	0.77%	0.085%
59	18.808	2640	2642	2646	rVB5	5240	7155	0.26%	0.028%
60	18.878	2650	2654	2656	rBV4	6380	9198	0.33%	0.037%
61	18.925	2660	2662	2667	rVB6	6840	6908	0.25%	0.028%
62	19.090	2684	2690	2695	rBV10	17083	30887	1.11%	0.123%
63	19.160	2697	2702	2706	rVV6	20980	30642	1.10%	0.122%
64	19.260	2715	2719	2723	rBV2	16114	20707	0.75%	0.082%
65	19.337	2725	2732	2734	rBV2	39781	70071	2.52%	0.279%
66	19.366	2734	2737	2740	rVV2	32963	44267	1.59%	0.176%
67	19.483	2753	2757	2767	rVB2	72529	98664	3.55%	0.393%
68	19.689	2787	2792	2800	rVB	1180129	1767038	63.65%	7.036%
69	19.754	2800	2803	2807	rVB	36707	43088	1.55%	0.172%
70	19.853	2817	2820	2824	rBV6	9046	9117	0.33%	0.036%
71	20.212	2878	2881	2884	rBV4	11639	13460	0.48%	0.054%
72	20.253	2884	2888	2891	rVB	14520	16352	0.59%	0.065%
73	20.570	2937	2942	2944	rBV6	11323	17804	0.64%	0.071%
74	20.676	2958	2960	2964	rVB4	10012	9775	0.35%	0.039%
75	20.717	2964	2967	2969	rBV3	12369	14574	0.52%	0.058%
76	20.740	2969	2971	2974	rVV2	13444	16669	0.60%	0.066%

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77	20.776	2974	2977	2980	rVB5	20174	22038	0.79%	0.088%
78	21.228	3049	3054	3062	rBV	232877	351095	12.65%	1.398%
79	21.551	3102	3109	3115	rBV	754351	1257705	45.30%	5.008%
80	21.774	3143	3147	3151	rBV	26251	37237	1.34%	0.148%
81	22.003	3181	3186	3191	rBV3	33347	49848	1.80%	0.198%
82	22.374	3244	3249	3260	rVB3	63664	146710	5.28%	0.584%
83	23.037	3356	3362	3368	rBV3	18571	40619	1.46%	0.162%
84	23.219	3389	3393	3400	rVB5	11978	22404	0.81%	0.089%
85	23.366	3413	3418	3425	rVB3	27908	54317	1.96%	0.216%
86	23.666	3462	3469	3474	rBV2	19222	48226	1.74%	0.192%
87	23.813	3488	3494	3499	rBV2	38084	78003	2.81%	0.311%
88	24.353	3580	3586	3588	rBV4	10077	20039	0.72%	0.080%
89	24.424	3588	3598	3619	rVB	708015	1935660	69.73%	7.707%
90	24.635	3623	3634	3644	rBV	480216	1327565	47.82%	5.286%
91	24.729	3646	3650	3659	rVB3	27439	63801	2.30%	0.254%
92	25.816	3827	3835	3844	rBV3	41075	122987	4.43%	0.490%
93	25.922	3848	3853	3863	rVB5	31140	90047	3.24%	0.359%
94	28.289	4247	4256	4268	rVB5	38357	155157	5.59%	0.618%
95	28.694	4308	4325	4342	rBV4	652167	2776091	100.00%	11.053%
96	29.529	4459	4467	4478	rBV4	26414	96163	3.46%	0.383%
97	29.746	4492	4504	4519	rVV4	84054	425735	15.34%	1.695%
98	30.134	4568	4570	4571	rBV2	6769	6488	0.23%	0.026%
99	31.820	4842	4857	4864	rBV2	56118	276291	9.95%	1.100%
100	32.401	4949	4956	4957	rBV7	11419	21498	0.77%	0.086%

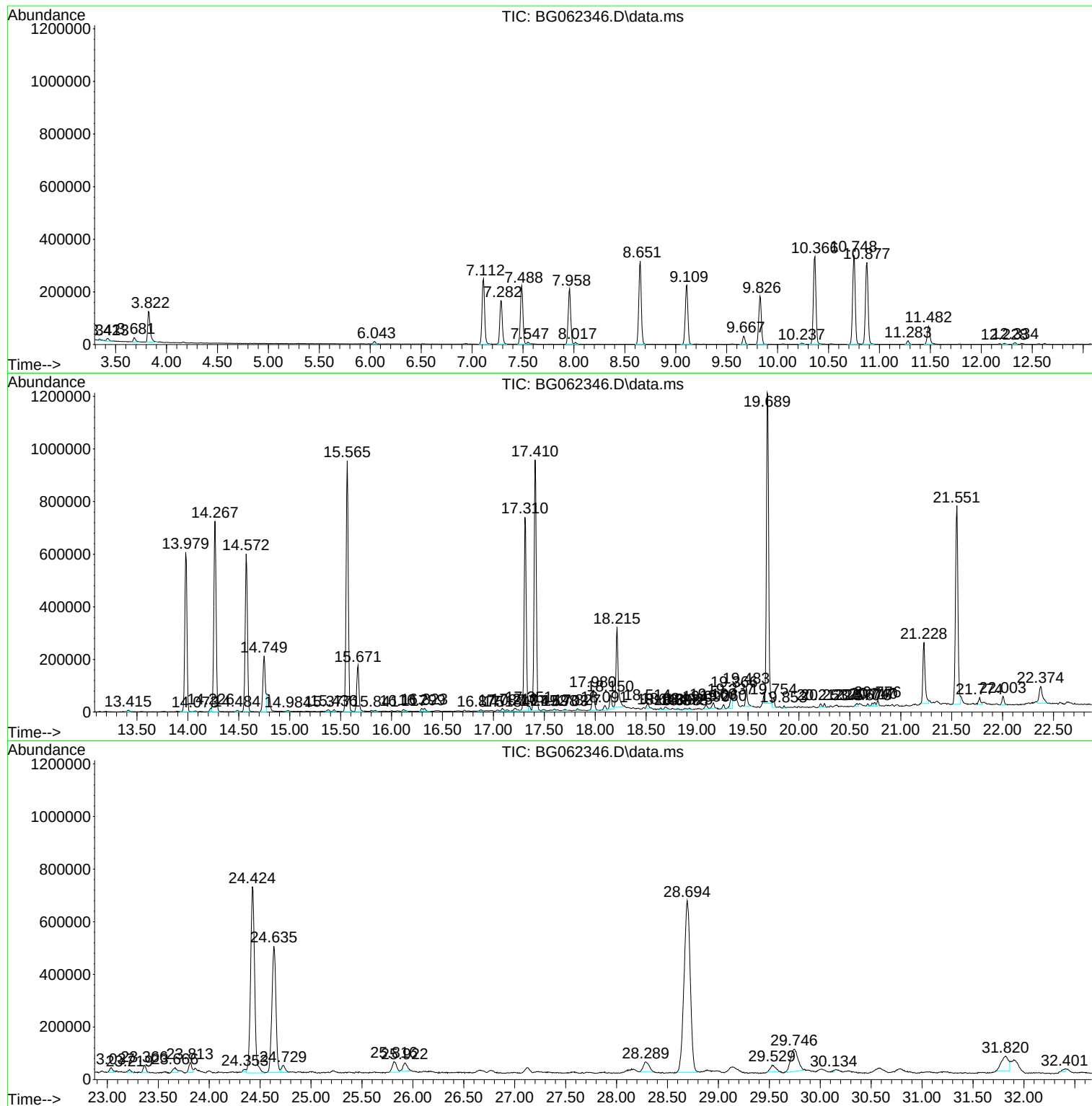
Sum of corrected areas: 25115475

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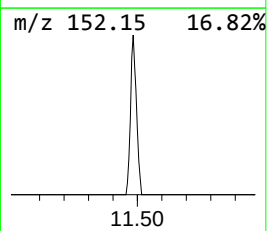
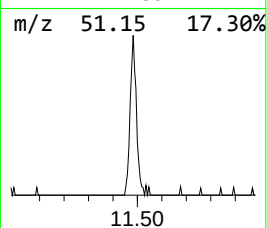
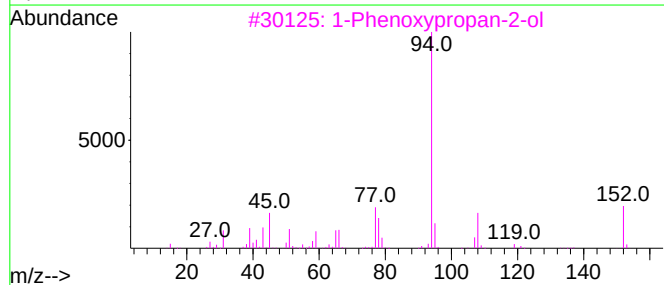
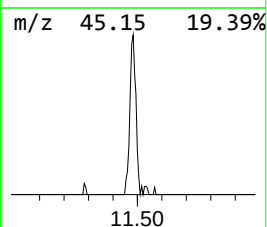
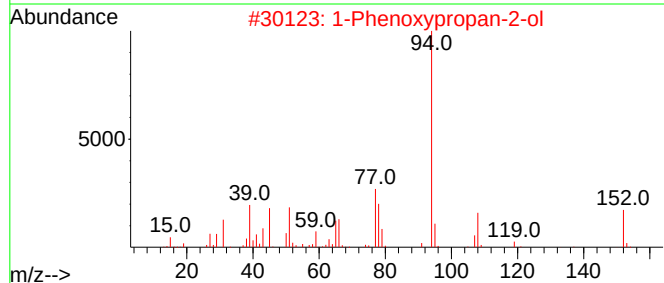
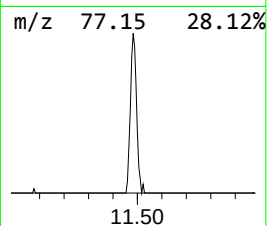
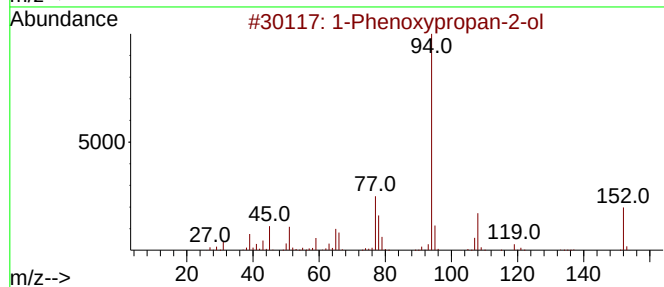
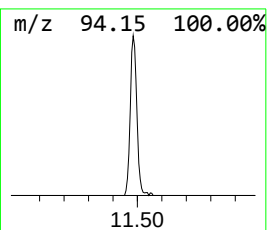
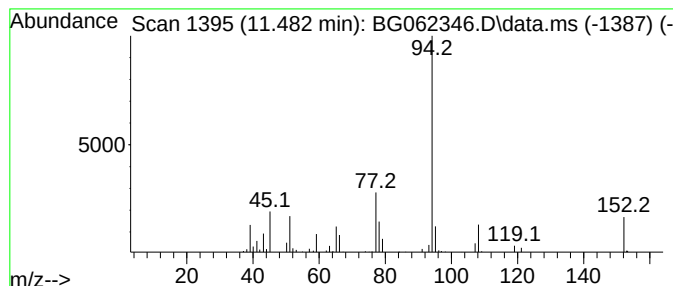
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.482	4.27 ng/ul	128385	Naphthalene-d8	10.748

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	94
3			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	93
4			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	90
5			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87



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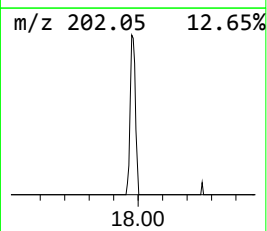
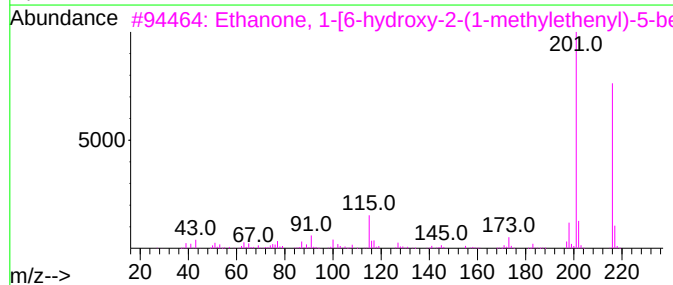
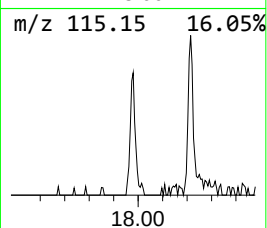
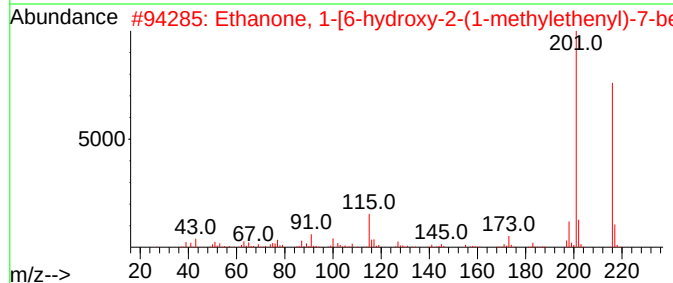
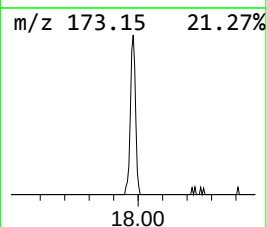
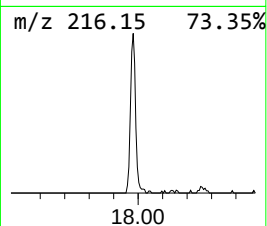
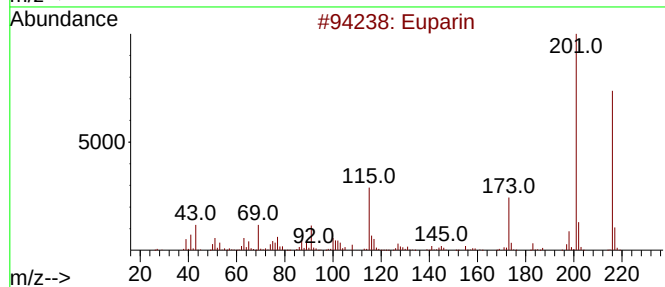
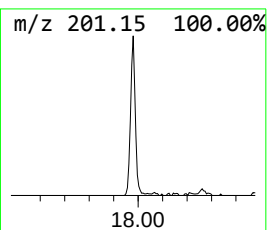
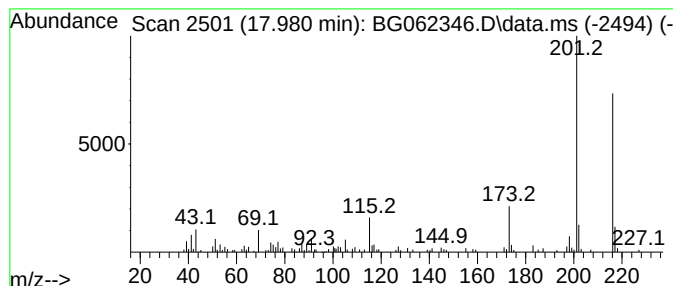
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Euparin Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	2.23 ng/ul	121943	Phenanthrene-d10	17.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Euparin	216	C13H12O3	000532-48-9	95
2			Ethanone, 1-[6-hydroxy-2-(1-meth...	216	C13H12O3	055682-75-2	87
3			Ethanone, 1-[6-hydroxy-2-(1-meth...	216	C14H16O2	1000414-89-5	87
4			1H-Pyrido[3,4-b]indole, 2,3,4,9-...	216	C13H16N2O	001210-56-6	64
5			1'-Acetonaphthone, 2'-hydroxy-4'...	216	C13H12O3	005891-63-4	64



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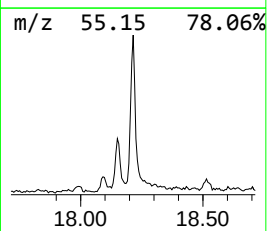
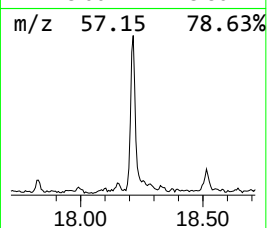
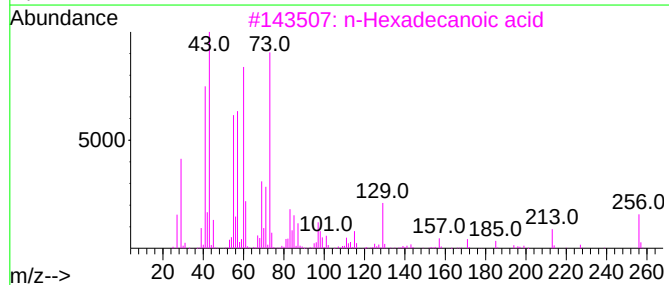
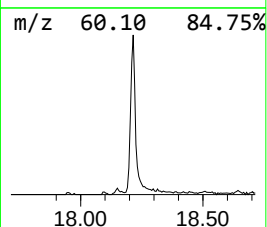
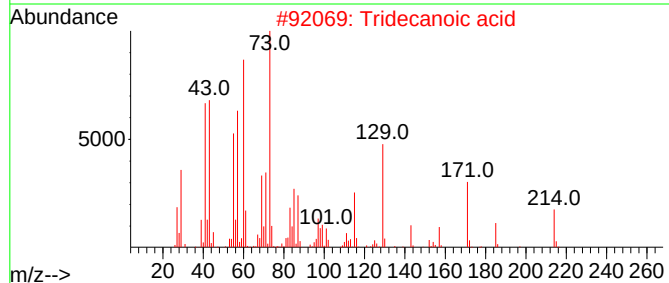
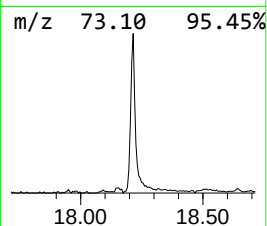
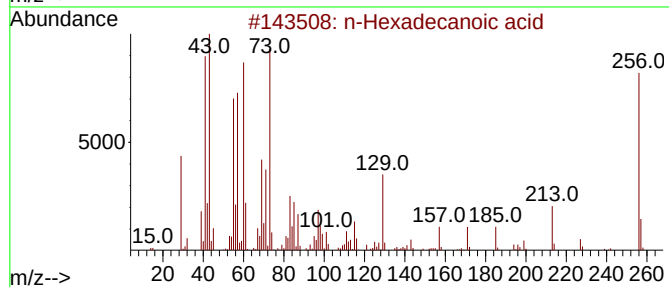
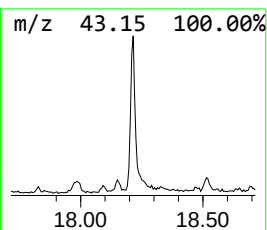
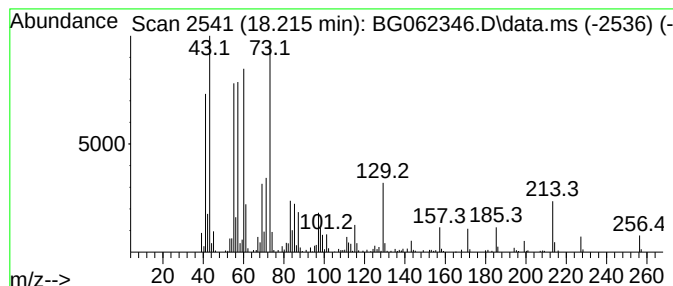
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.215	8.06 ng/ul	440024	Phenanthrene-d10	17.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98		
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93		
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87		
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87		
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062346.D
Acq On : 9 Aug 2024 3:51
Operator : MA/JU
Sample : P3434-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05T5

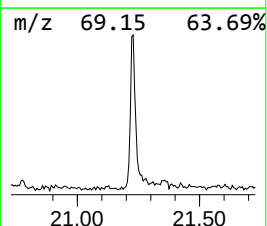
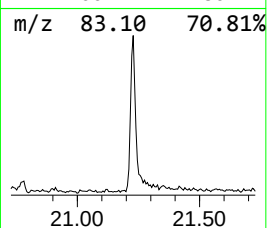
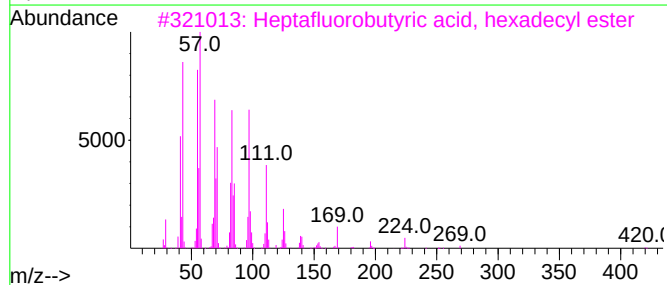
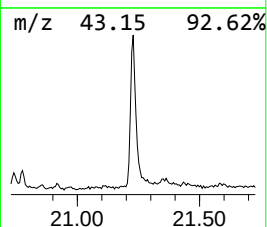
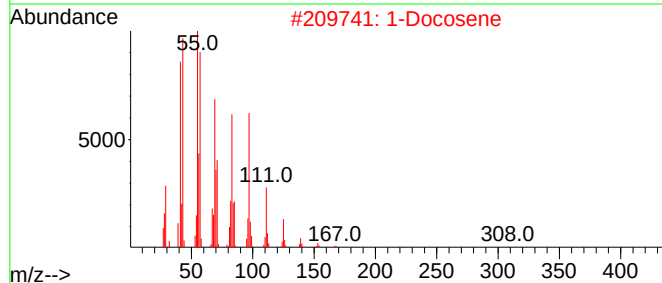
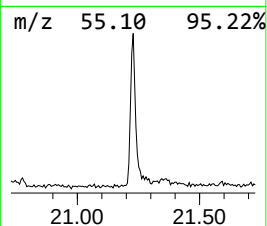
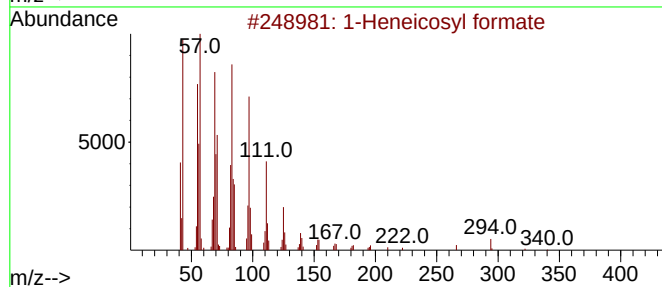
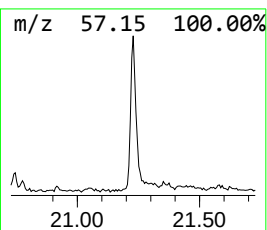
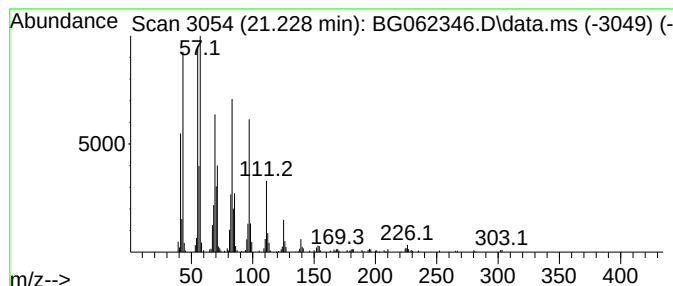
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.228	5.58 ng/ul	351095	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2			1-Docosene	308	C22H44	001599-67-3	94
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062346.D
Acq On : 9 Aug 2024 3:51
Operator : MA/JU
Sample : P3434-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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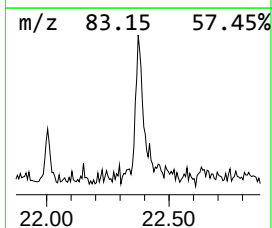
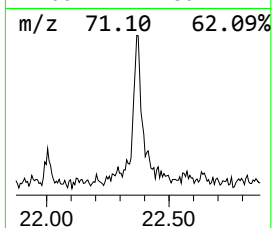
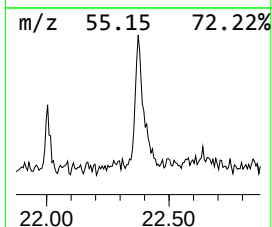
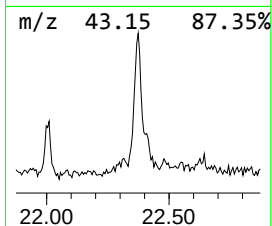
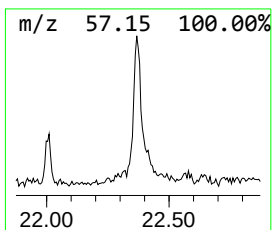
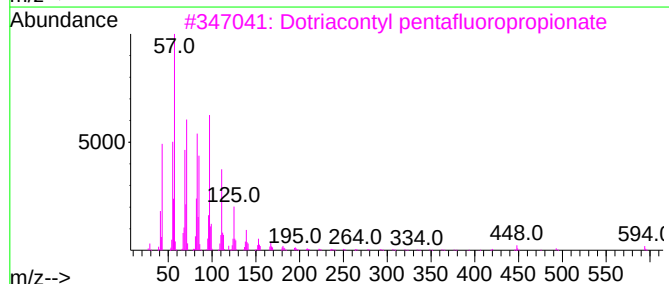
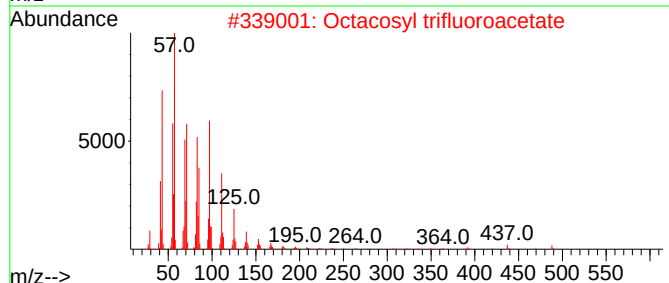
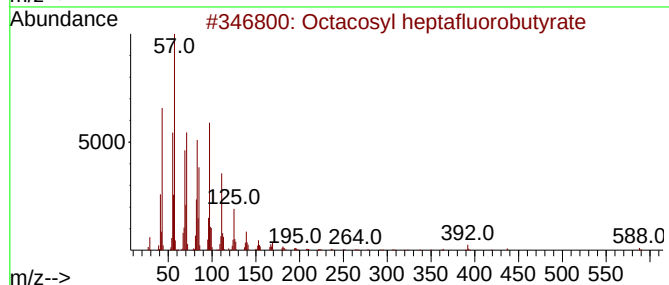
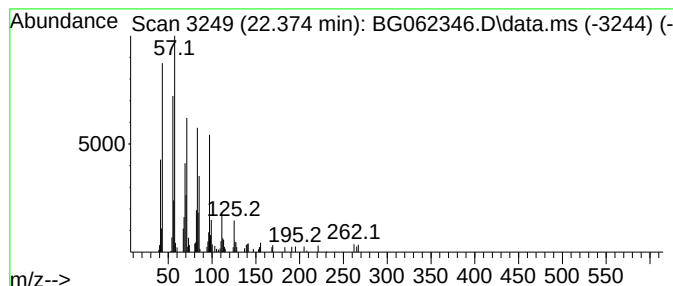
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Octacosyl heptafluorobutyrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.374	2.33 ng/ul	146710	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	83
2			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	80
3			Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	80
4			Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	72
5			Isobutyl tetracosyl ether	410	C28H58O	1000406-33-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062346.D
Acq On : 9 Aug 2024 3:51
Operator : MA/JU
Sample : P3434-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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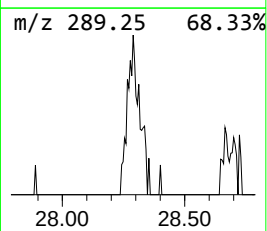
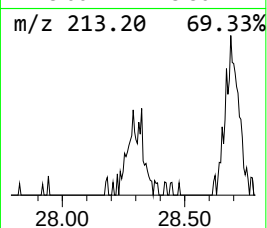
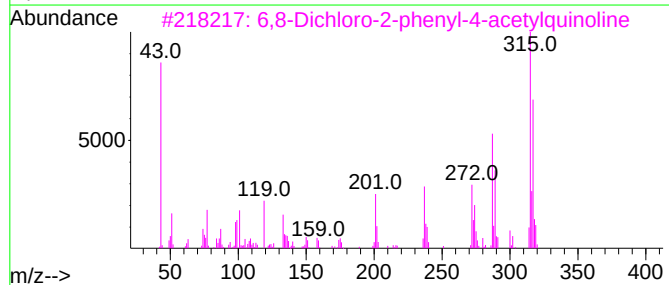
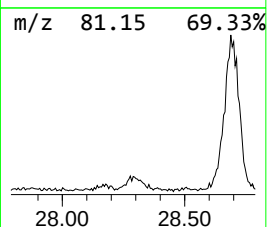
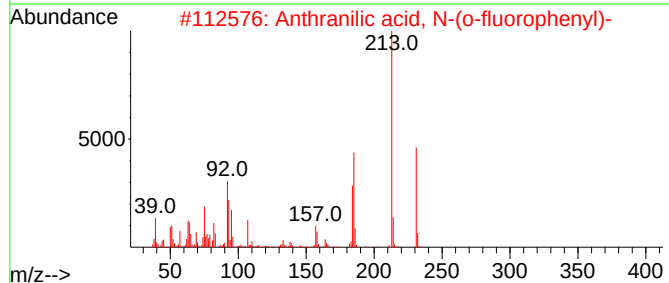
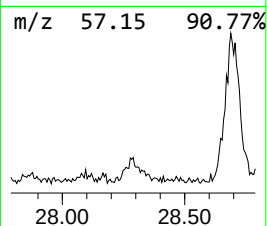
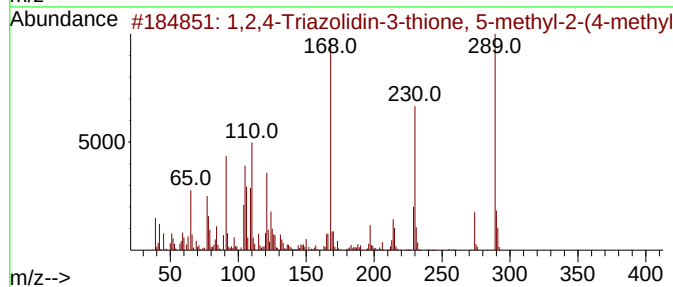
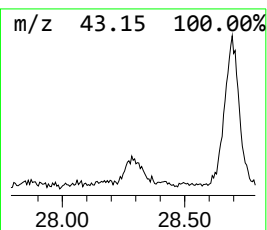
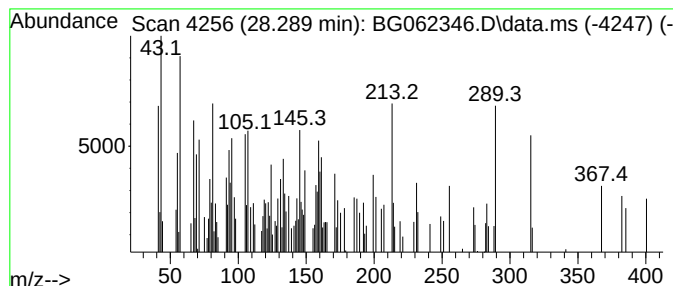
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.289	2.34 ng/ul	155157	Perylene-d12	24.635

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Triazolidin-3-thione, 5-me...	289	C14H15N3S2	346459-14-1	15
2			Anthranilic acid, N-(o-fluorophe...	231	C13H10FNO2	000054-58-0	11
3			6,8-Dichloro-2-phenyl-4-acetylqu...	315	C17H11Cl2NO	1000255-89-3	10
4			Trihexyl 2-(butyryloxy)propane-1...	514	C28H50O8	082469-79-2	10
5			4-Hydrazino-8-methyl-5H-pyrimido...	213	C11H11N5	1000459-89-7	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062346.D
Acq On : 9 Aug 2024 3:51
Operator : MA/JU
Sample : P3434-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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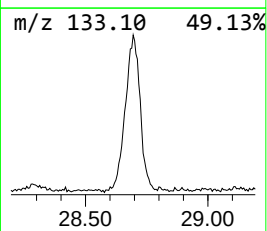
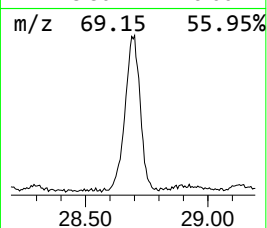
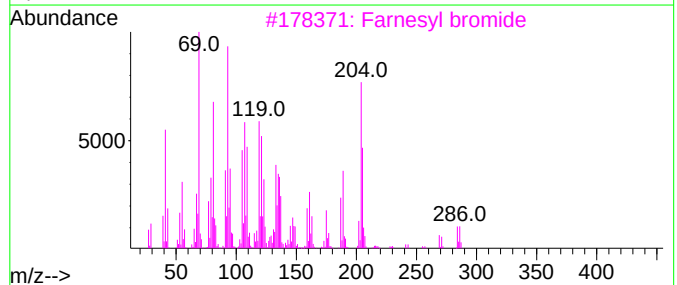
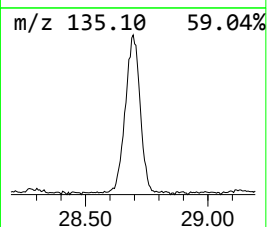
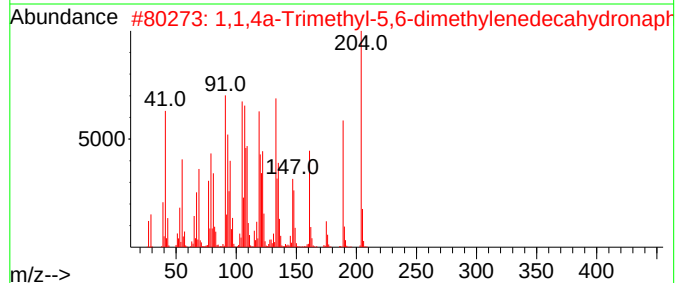
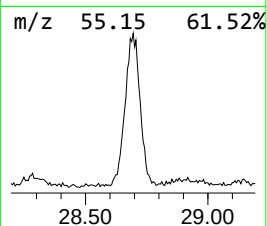
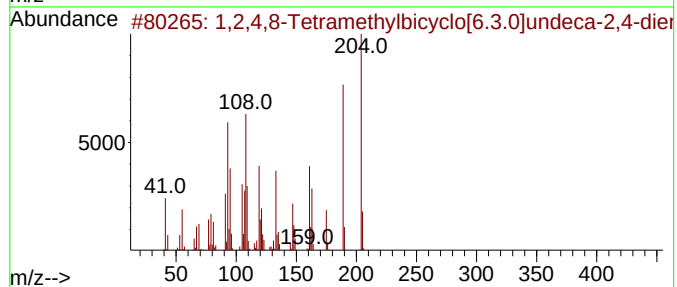
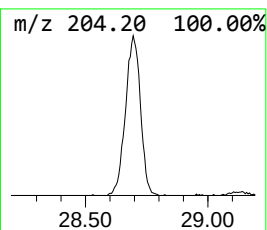
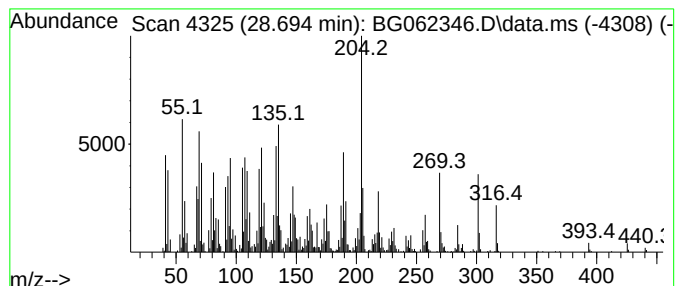
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 1,2,4,8-Tetramethylbicyclo[... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.694	41.82 ng/ul	2776090	Perylene-d12	24.635

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	78		
2	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	76		
3	Farnesyl bromide	284	C15H25Br	006874-67-5	55		
4	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	46		
5	1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062346.D
Acq On : 9 Aug 2024 3:51
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Sample : P3434-04
Misc :
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Instrument :
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ClientSampleId :
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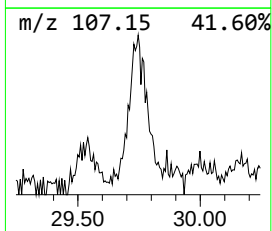
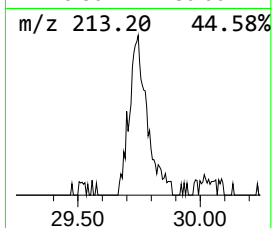
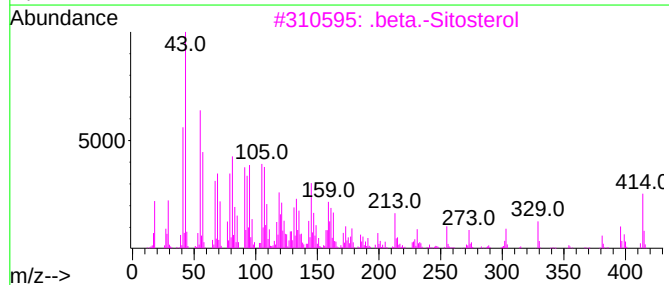
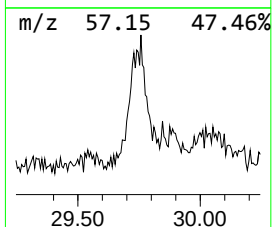
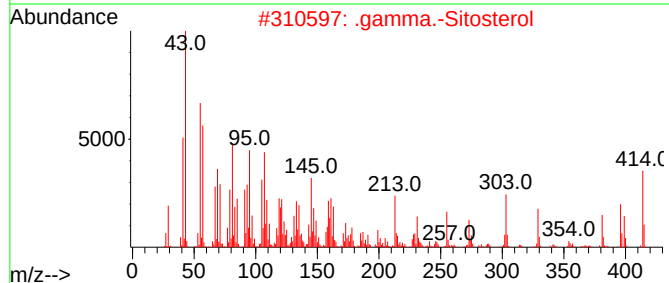
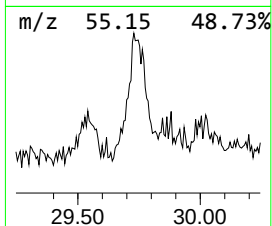
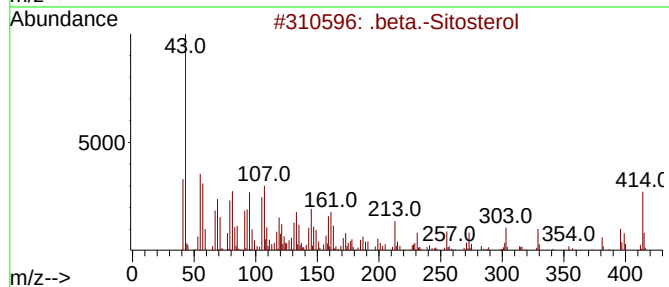
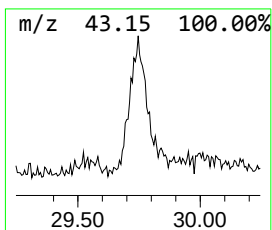
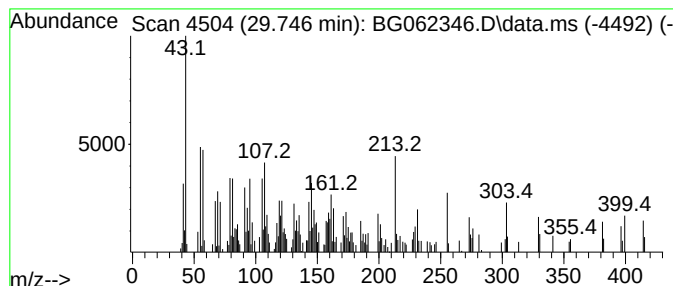
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 .beta.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.746	6.41 ng/ul	425735	Perylene-d12	24.635

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	beta.-Sitosterol	414	C29H50O	000083-46-5	91	
2	.	gamma.-Sitosterol	414	C29H50O	000083-47-6	87	
3	.	beta.-Sitosterol	414	C29H50O	000083-46-5	42	
4	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	42		
5	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	35		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
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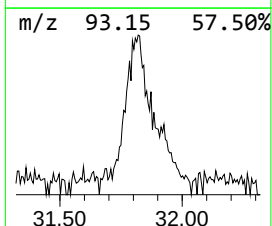
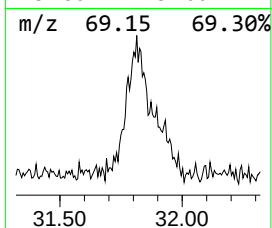
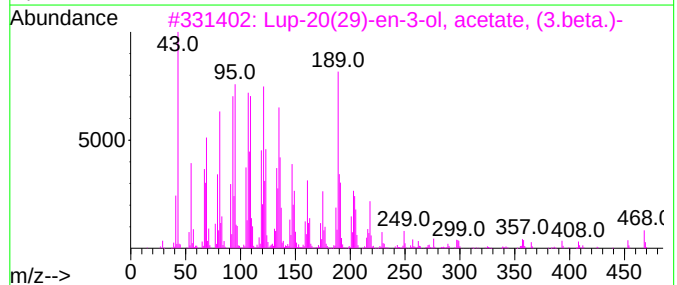
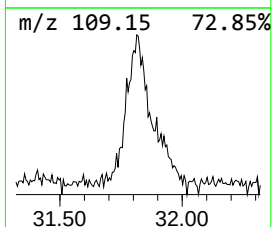
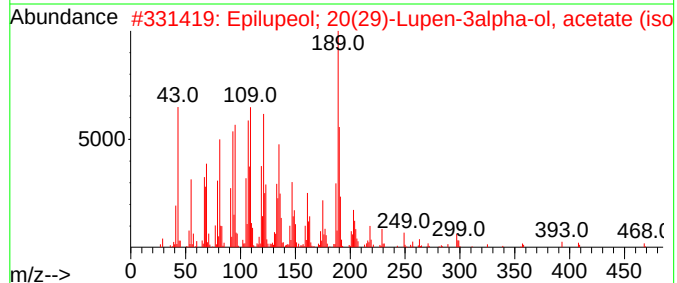
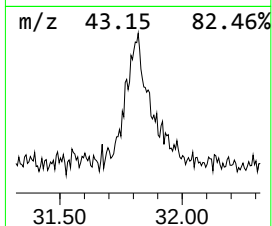
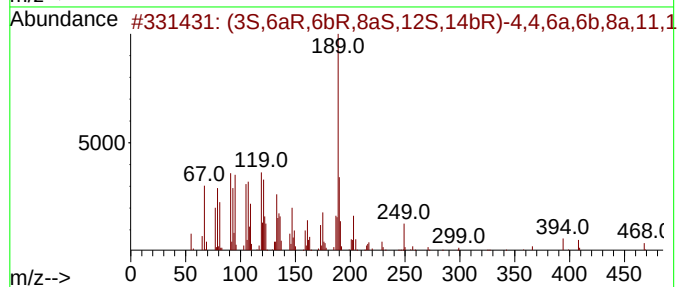
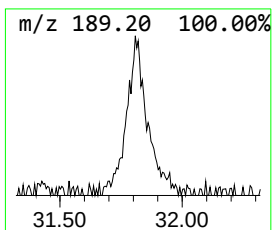
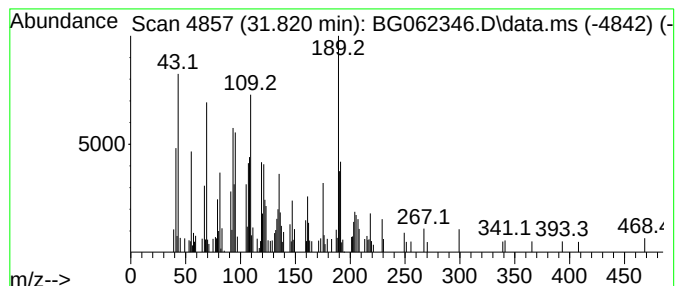
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 9 (3S,6aR,6bR,8aS,12S,14bR)-4... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
31.820	4.16 ng/ul	276291	Perylene-d12	24.635	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3S,6aR,6bR,8aS,12S,14bR)-4,4,6a...	468	C32H52O2	1000441-99-9	90
2	Epilupeol; 20(29)-Lupen-3alpha-o...	468	C32H52O2	1010513-01-8	83
3	Lup-20(29)-en-3-ol, acetate, (3...	468	C32H52O2	001617-68-1	58
4	(3S,3aR,6R,8aS)-7,7-Dimethyl-8-m...	218	C15H22O	082509-29-3	50
5	(1aR,4S,4aR,7R,7aS,7bS)-1,1,4,7-...	222	C15H26O	088728-58-9	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062346.D
Acq On : 9 Aug 2024 3:51
Operator : MA/JU
Sample : P3434-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
1-Phenoxypropan...	11.482	4.3	ng/ul	128385	2	10.748	600685	20.0
Euparin	17.980	2.2	ng/ul	121943	4	17.310	1092380	20.0
n-Hexadecanoic ...	18.215	8.1	ng/ul	440024	4	17.310	1092380	20.0
1-Heneicosyl fo...	21.228	5.6	ng/ul	351095	5	21.551	1257710	20.0
Octacosyl hepta...	22.374	2.3	ng/ul	146710	5	21.551	1257710	20.0
unknown-01	28.289	2.3	ng/ul	155157	6	24.635	1327570	20.0
1,2,4,8-Tetrame...	28.694	41.8	ng/ul	2776090	6	24.635	1327570	20.0
.beta.-Sitosterol	29.746	6.4	ng/ul	425735	6	24.635	1327570	20.0
(3S,6aR,6bR,8aS...	31.820	4.2	ng/ul	276291	6	24.635	1327570	20.0