

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012422\
 Data File : BG052125.D
 Acq On : 24 Jan 2022 14:20
 Operator : CG/JU
 Sample : N1199-17
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0Q12

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-BG010622.M
 Title : SVOA CALIBRATION

Signal : TIC: BG052125.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.572	10	14	20	rVB	5650	7879	0.75%	0.078%
2	3.848	59	61	66	rBV3	2798	3301	0.31%	0.033%
3	4.001	83	87	97	rBV2	23547	42526	4.04%	0.423%
4	4.347	143	146	151	rBV2	2652	3440	0.33%	0.034%
5	6.503	509	513	522	rVB4	3741	6684	0.64%	0.066%
6	7.384	655	663	671	rVB2	33145	60815	5.78%	0.605%
7	7.549	685	691	699	rBB	106779	175665	16.70%	1.747%
8	7.772	721	729	736	rBV2	105693	190466	18.10%	1.895%
9	8.242	802	809	816	rBV	95436	158684	15.08%	1.579%
10	8.947	922	929	938	rBV	97425	164613	15.64%	1.637%
11	9.411	998	1008	1017	rBV	144802	265603	25.24%	2.642%
12	9.834	1074	1080	1085	rBV2	7470	11002	1.05%	0.109%
13	10.145	1126	1133	1141	rBV	126560	226548	21.53%	2.254%
14	10.327	1162	1164	1170	rBV	1550	1767	0.17%	0.018%
15	10.697	1219	1227	1239	rVB	186727	332927	31.64%	3.312%
16	10.827	1244	1249	1257	rVB2	8546	15642	1.49%	0.156%
17	11.085	1285	1293	1300	rBV	131527	238229	22.64%	2.370%
18	11.208	1306	1314	1323	rBV	127782	242045	23.00%	2.408%
19	12.330	1498	1505	1511	rVB2	9139	12704	1.21%	0.126%
20	12.653	1554	1560	1566	rVB3	3961	5715	0.54%	0.057%
21	13.323	1670	1674	1676	rBV2	2109	2586	0.25%	0.026%
22	13.699	1733	1738	1741	rBV2	3003	4406	0.42%	0.044%
23	13.764	1741	1749	1757	rVB	46328	73150	6.95%	0.728%
24	14.275	1830	1836	1845	rVB	372138	548538	52.13%	5.457%
25	14.504	1873	1875	1881	rVB3	1454	1769	0.17%	0.018%
26	14.586	1881	1889	1896	rVB	407907	656960	62.44%	6.535%
27	14.768	1915	1920	1923	rVB2	1782	2521	0.24%	0.025%
28	14.886	1934	1940	1947	rBV	229770	361591	34.37%	3.597%
29	15.074	1965	1972	1983	rBV	28535	52904	5.03%	0.526%
30	15.215	1992	1996	1997	rBV2	1617	1537	0.15%	0.015%
31	15.661	2066	2072	2076	rBV2	1512	2519	0.24%	0.025%
32	15.714	2076	2081	2083	rVB3	1729	2563	0.24%	0.025%
33	15.879	2100	2109	2115	rBV	552130	823219	78.24%	8.189%
34	15.984	2121	2127	2136	rBV2	166562	244844	23.27%	2.436%
35	16.125	2145	2151	2155	rBV3	2971	4549	0.43%	0.045%
36	16.572	2224	2227	2230	rVB2	1715	1820	0.17%	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

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-BG010622.M
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37	16.754	2254	2258	2260	rBV3	1507	1901	0.18%	0.019%
38	16.789	2262	2264	2272	rVB2	866	1547	0.15%	0.015%
39	17.100	2311	2317	2320	rBV2	5740	7813	0.74%	0.078%
40	17.147	2323	2325	2330	rVB2	978	1628	0.15%	0.016%
41	17.371	2358	2363	2368	rBV4	4192	5481	0.52%	0.055%
42	17.424	2368	2372	2374	rBV3	2712	3797	0.36%	0.038%
43	17.641	2401	2409	2414	rBV	287785	448189	42.60%	4.458%
44	17.735	2419	2425	2435	rVB	585993	906325	86.14%	9.016%
45	17.846	2442	2444	2449	rVB4	1373	1831	0.17%	0.018%
46	17.993	2466	2469	2470	rBV3	2918	3285	0.31%	0.033%
47	18.023	2473	2474	2478	rVV4	2160	2725	0.26%	0.027%
48	18.111	2485	2489	2494	rVB3	6014	6578	0.63%	0.065%
49	18.181	2494	2501	2505	rBV2	6622	11443	1.09%	0.114%
50	18.281	2514	2518	2523	rVB2	40088	46425	4.41%	0.462%
51	18.504	2552	2556	2559	rBV5	3638	5498	0.52%	0.055%
52	18.610	2573	2574	2577	rBV3	2136	2585	0.25%	0.026%
53	18.692	2586	2588	2589	rBV2	2368	1574	0.15%	0.016%
54	18.798	2603	2606	2609	rBV2	5632	6200	0.59%	0.062%
55	18.898	2621	2623	2626	rBV3	2131	2261	0.21%	0.022%
56	19.109	2654	2659	2664	rBV4	9193	13310	1.26%	0.132%
57	19.198	2672	2674	2675	rBV2	1957	1675	0.16%	0.017%
58	19.438	2707	2715	2720	rBV	120494	156421	14.87%	1.556%
59	19.574	2733	2738	2745	rVB2	38471	51136	4.86%	0.509%
60	19.650	2747	2751	2754	rBV2	9248	14583	1.39%	0.145%
61	19.679	2754	2756	2763	rVB3	14743	19623	1.86%	0.195%
62	19.867	2787	2788	2789	rBV	3529	1785	0.17%	0.018%
63	19.897	2790	2793	2799	rVB2	14879	20981	1.99%	0.209%
64	20.014	2807	2813	2822	rVB	696252	1052198	100.00%	10.467%
65	20.519	2897	2899	2900	rBV	4363	2863	0.27%	0.028%
66	20.590	2907	2911	2913	rVB2	17738	20879	1.98%	0.208%
67	20.625	2915	2917	2922	rVB6	8147	8113	0.77%	0.081%
68	21.242	3019	3022	3031	rVB	20526	27805	2.64%	0.277%
69	21.559	3073	3076	3081	rBV6	10931	20180	1.92%	0.201%
70	21.959	3137	3144	3150	rBV	282848	501701	47.68%	4.991%
71	22.775	3280	3283	3289	rVB5	16696	27650	2.63%	0.275%
72	23.556	3412	3416	3421	rVB7	10222	14525	1.38%	0.144%
73	23.762	3442	3451	3458	rVB	68149	166859	15.86%	1.660%
74	25.207	3686	3697	3712	rVB2	337013	1009229	95.92%	10.039%
75	25.448	3728	3738	3753	rVB2	157770	495989	47.14%	4.934%
76	28.843	4314	4316	4317	rBV	3169	1619	0.15%	0.016%

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ClientSampleId :
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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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Title : SVOA CALIBRATION

77	30.277	4558	4560	4562	rBV2	3255	2838	0.27%	0.028%
78	31.692	4799	4801	4802	rBV2	2980	1949	0.19%	0.019%

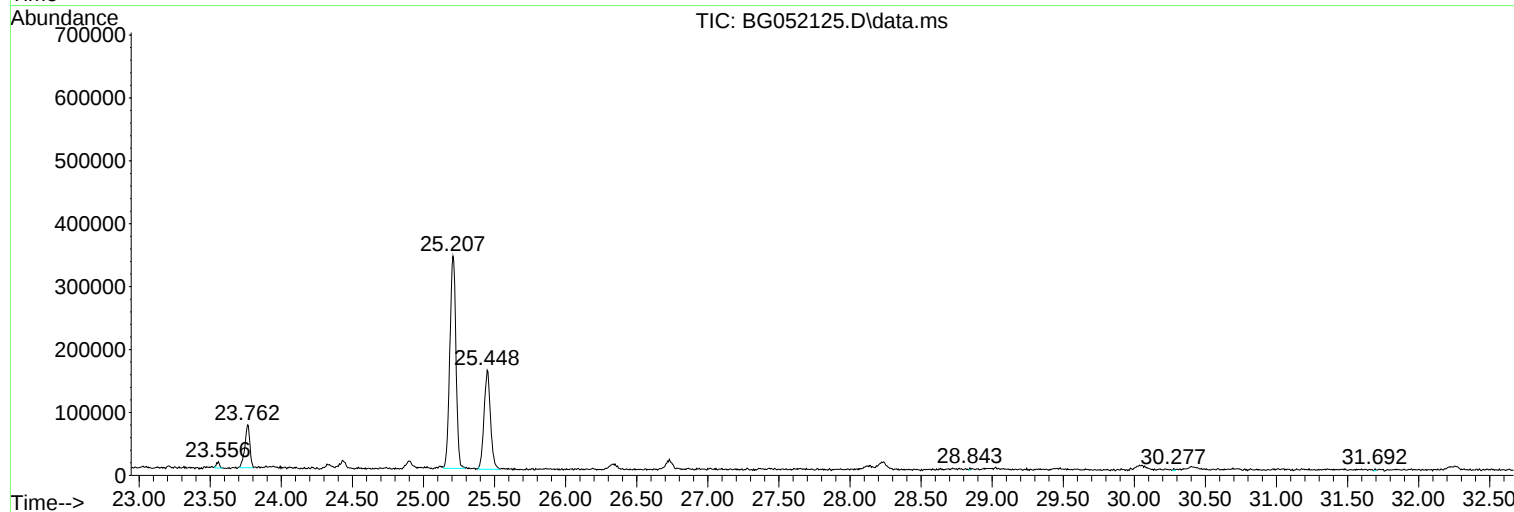
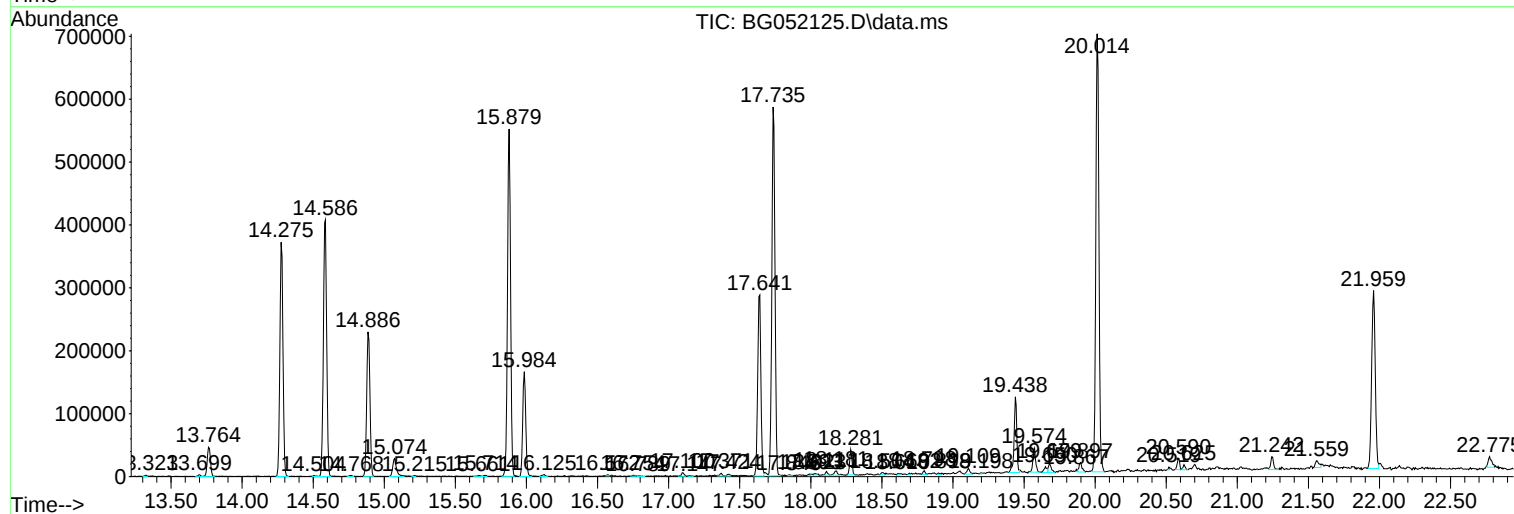
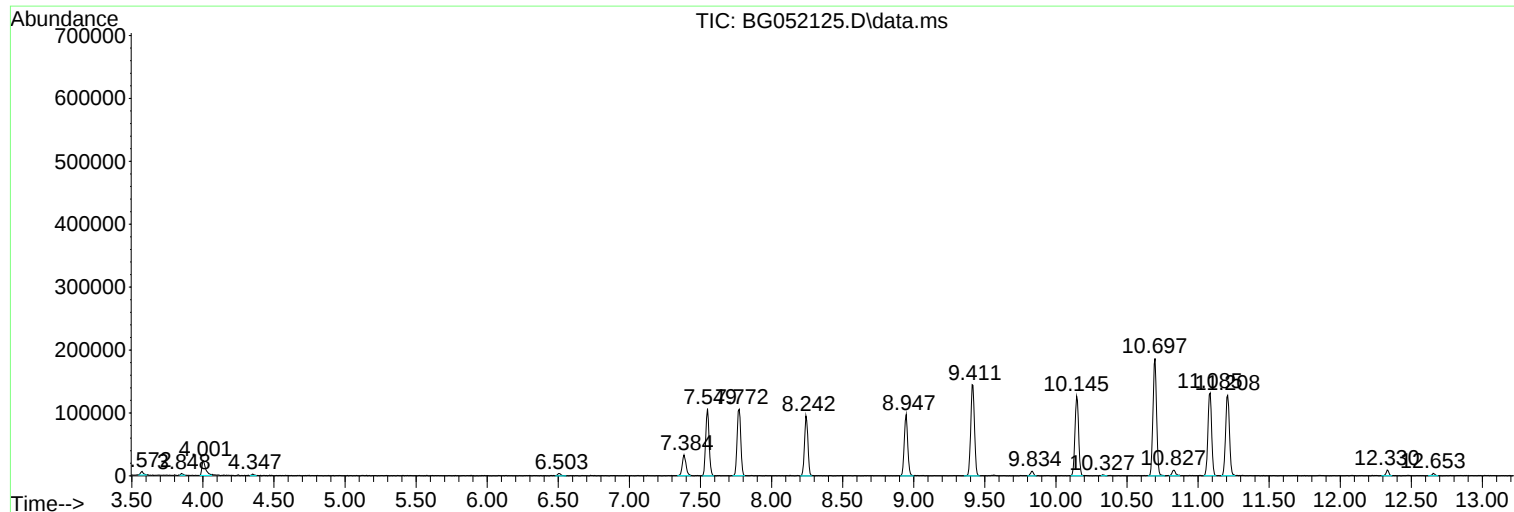
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.M
Quant Title : SVOA CALIBRATION

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



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Operator : CG/JU
Sample : N1199-17
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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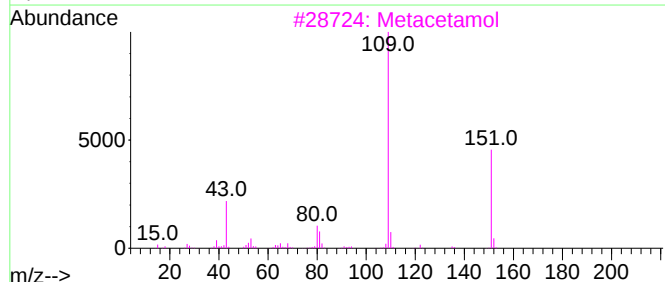
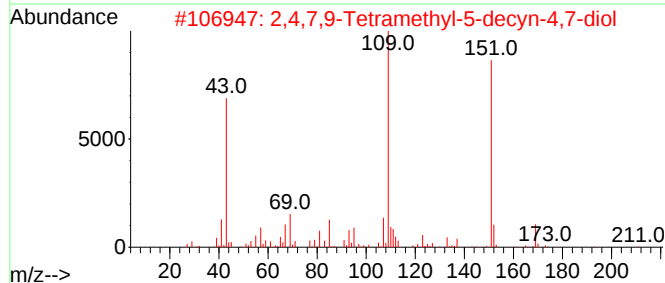
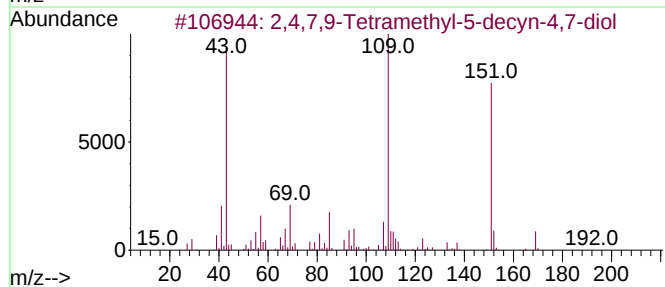
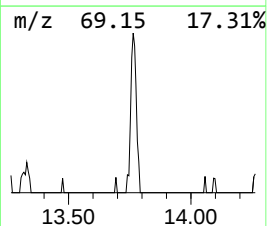
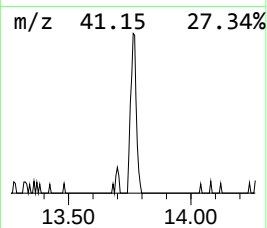
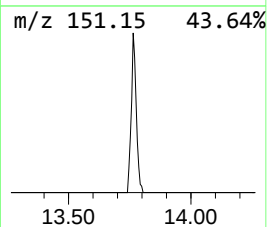
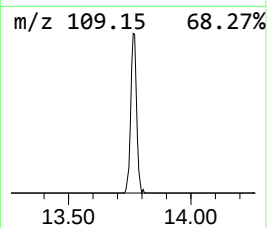
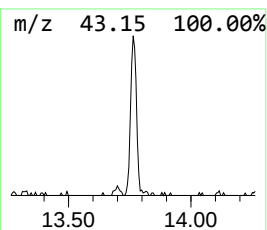
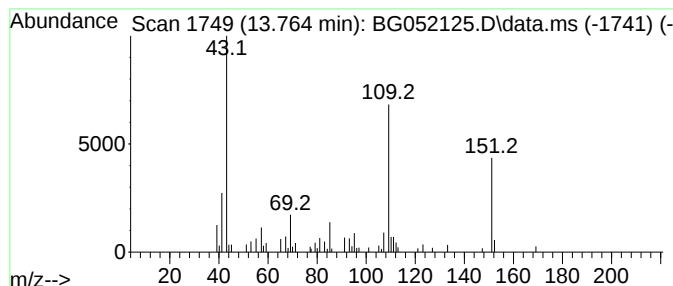
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.764	4.05 ng/ul	73150	Acenaphthene-d10	14.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91		
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90		
3	Metacetamol	151	C8H9NO2	000621-42-1	53		
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	42		
5	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	42		



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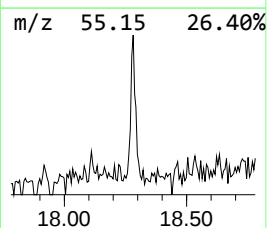
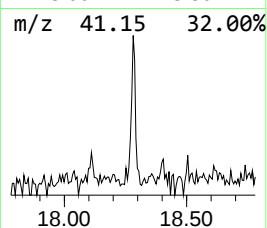
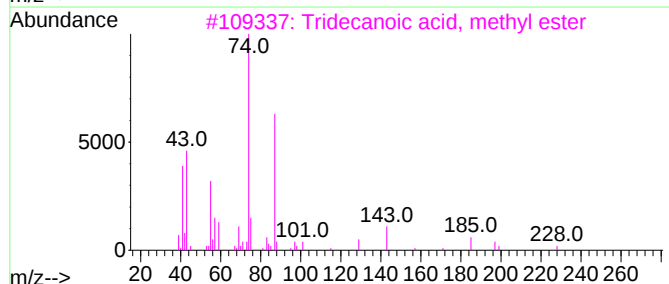
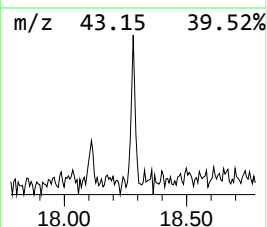
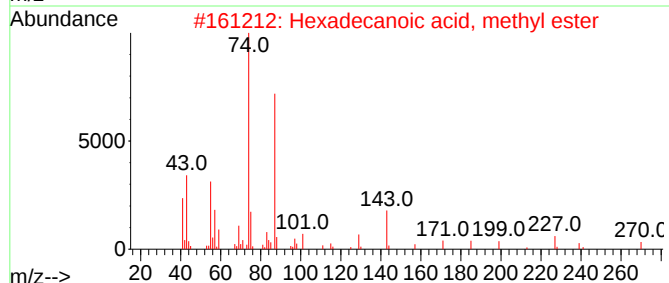
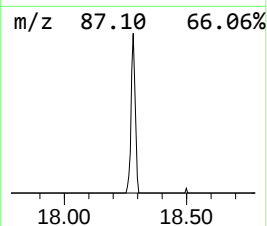
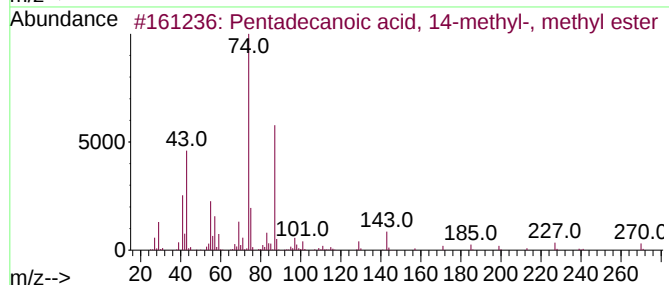
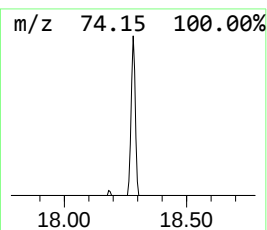
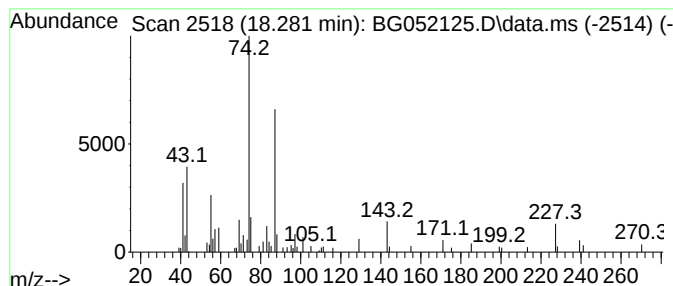
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Pentadecanoic acid, 14-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.281	2.07 ng/ul	46425	Phenanthrene-d10	17.641

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
2			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	87
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	80



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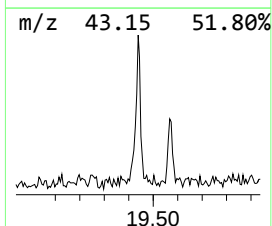
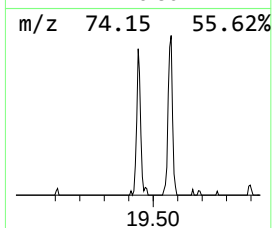
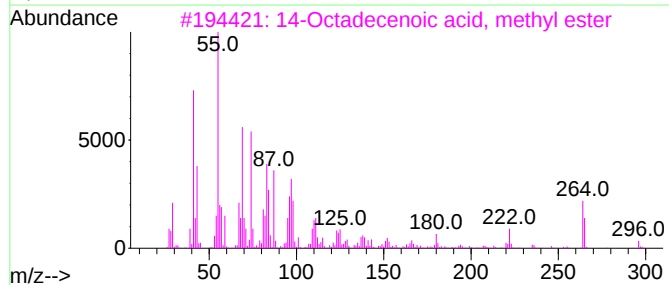
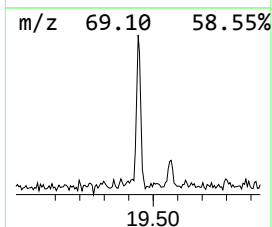
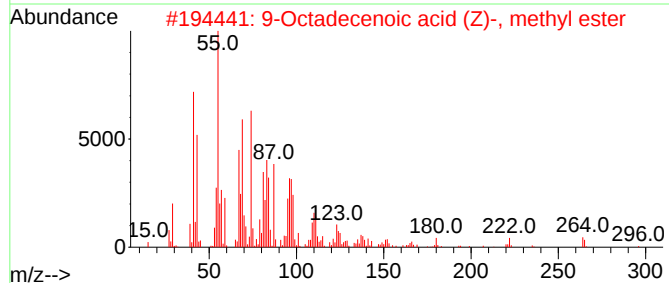
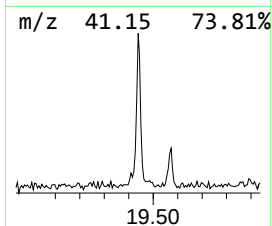
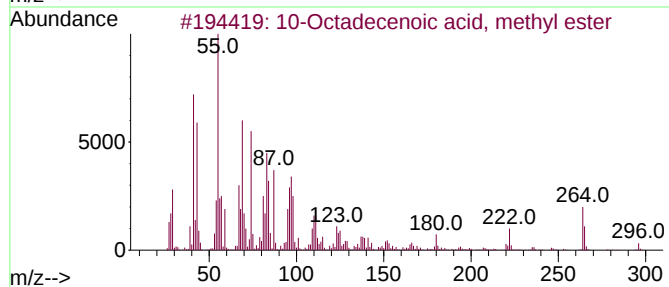
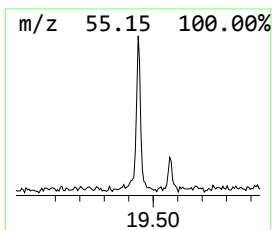
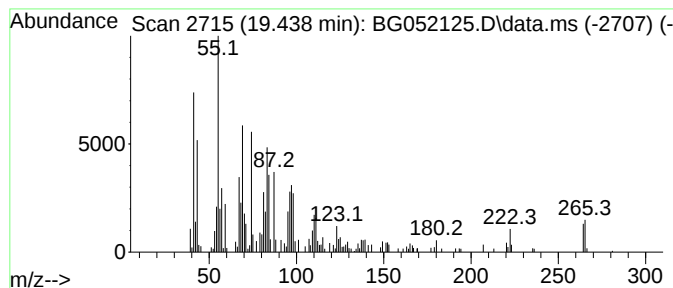
Instrument :
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 10-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.438	6.98 ng/ul	156421	Phenanthrene-d10		17.641	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester		296	C19H36O2	013481-95-3	94
2	9-Octadecenoic acid (Z)-, methyl...		296	C19H36O2	000112-62-9	93
3	14-Octadecenoic acid, methyl ester		296	C19H36O2	056554-48-4	91
4	15-Octadecenoic acid, methyl ester		296	C19H36O2	004764-72-1	91
5	13-Octadecenoic acid, methyl ester		296	C19H36O2	056554-47-3	86



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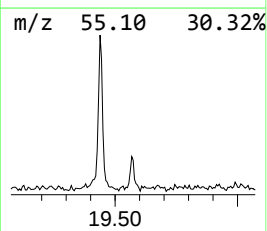
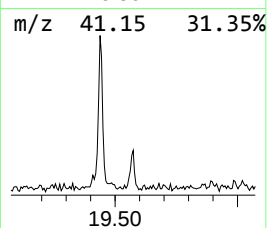
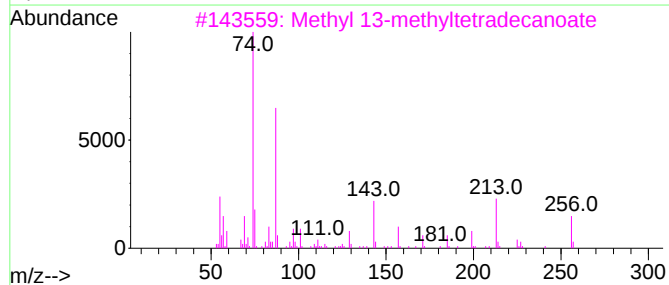
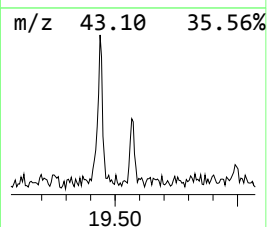
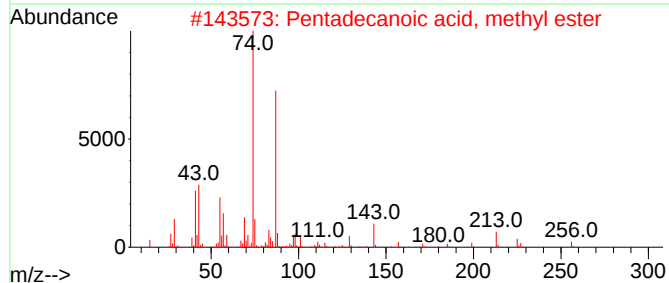
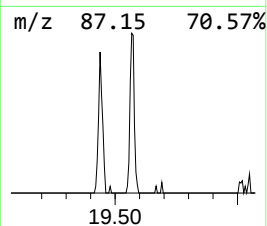
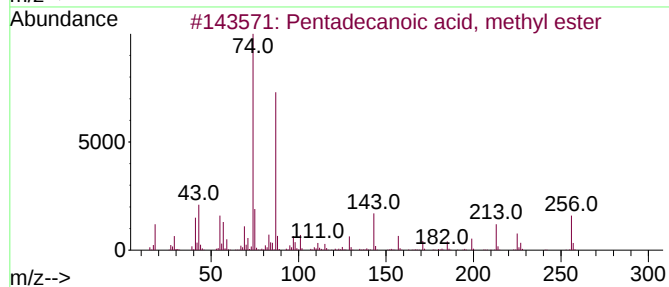
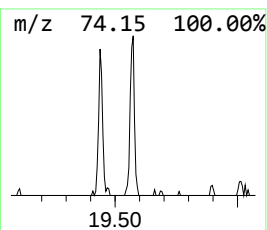
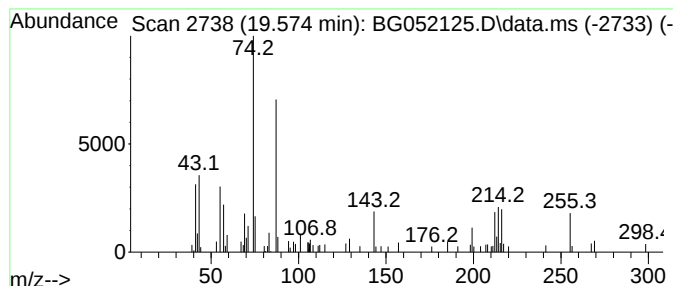
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Pentadecanoic acid, methyl ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.573	2.28 ng/ul	51136	Phenanthrene-d10	17.641

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	60
2			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	60
3			Methyl 13-methyltetradecanoate	256	C16H32O2	1000424-50-7	49
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	49
5			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012422\
Data File : BG052125.D
Acq On : 24 Jan 2022 14:20
Operator : CG/JU
Sample : N1199-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0Q12

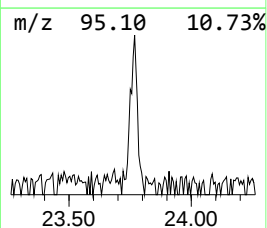
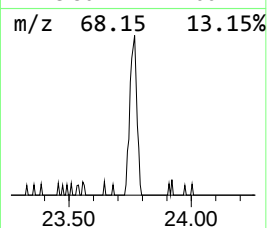
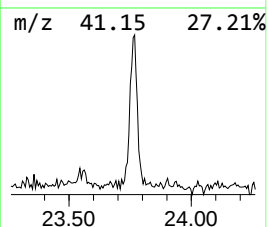
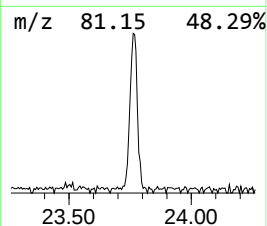
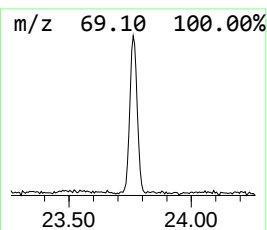
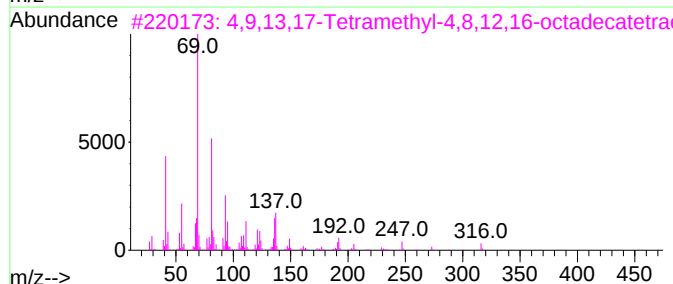
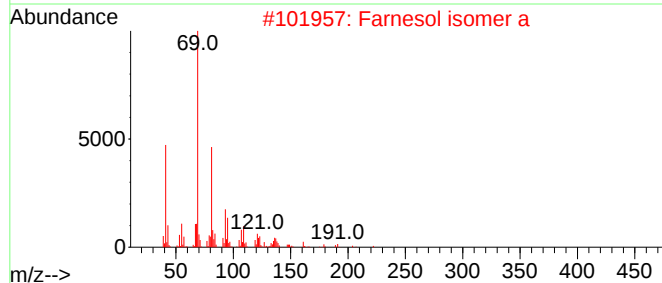
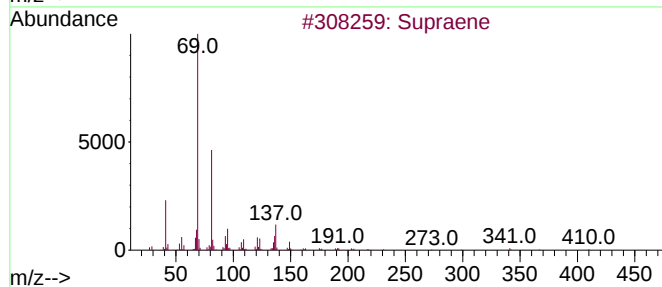
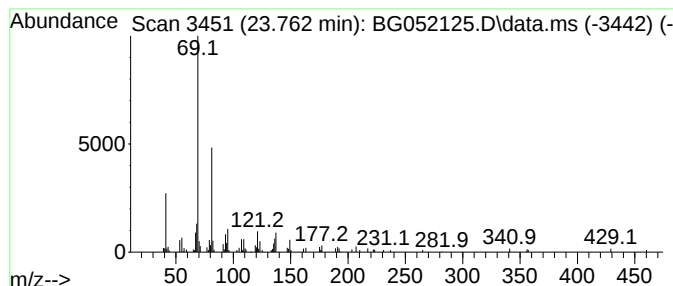
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.762	6.73 ng/ul	166859	Perylene-d12	25.448

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			Farnesol isomer a	222	C15H26O	1000108-92-4	74
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
4			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
5			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012422\
Data File : BG052125.D
Acq On : 24 Jan 2022 14:20
Operator : CG/JU
Sample : N1199-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0Q12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010622.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
2,4,7,9-Tetrame...	13.764	4.0	ng/ul	73150	3	14.886	361591	20.0
Pentadecanoic a...	18.281	2.1	ng/ul	46425	4	17.641	448189	20.0
10-Octadecenoic...	19.438	7.0	ng/ul	156421	4	17.641	448189	20.0
Pentadecanoic a...	19.573	2.3	ng/ul	51136	4	17.641	448189	20.0
Supraene	23.762	6.7	ng/ul	166859	6	25.448	495989	20.0