

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092023\
 Data File : BG059149.D
 Acq On : 21 Sep 2023 21:27
 Operator : MA/JU
 Sample : 04386-06
 Misc :
 ALS Vial : 50 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0AB9

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-BG091923.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG059149.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.040	107	111	121	rBV	79747	125482	17.90%	1.523%
2	4.252	146	147	152	rVB3	3916	2956	0.42%	0.036%
3	4.892	252	256	259	rBV3	1367	2163	0.31%	0.026%
4	5.309	322	327	334	rBV4	2445	4964	0.71%	0.060%
5	6.913	596	600	605	rBV2	4929	5439	0.78%	0.066%
6	7.407	675	684	694	rBV	88956	160287	22.86%	1.945%
7	7.612	712	719	727	rBV	94606	161554	23.04%	1.960%
8	7.689	727	732	738	rBV4	3413	6473	0.92%	0.079%
9	7.806	745	752	759	rBV2	100761	176072	25.11%	2.137%
10	8.294	828	835	843	rVB	95778	164633	23.48%	1.998%
11	8.476	861	866	870	rBV3	7373	9348	1.33%	0.113%
12	8.547	875	878	883	rVB2	1274	2215	0.32%	0.027%
13	8.975	945	951	958	rBV2	115926	194291	27.71%	2.358%
14	9.492	1030	1039	1051	rVB	115515	200966	28.66%	2.439%
15	10.209	1154	1161	1168	rBV	88496	153988	21.96%	1.869%
16	10.732	1243	1250	1257	rVB2	129980	227487	32.44%	2.761%
17	11.138	1311	1319	1326	rBV	142680	252406	36.00%	3.063%
18	11.279	1336	1343	1351	rBV	113720	205173	29.26%	2.490%
19	12.695	1577	1584	1587	rBV	2734	3683	0.53%	0.045%
20	13.188	1666	1668	1671	rVB	3507	2203	0.31%	0.027%
21	13.500	1718	1721	1725	rVB	1544	2256	0.32%	0.027%
22	13.752	1759	1764	1769	rBV3	13829	21325	3.04%	0.259%
23	14.081	1818	1820	1824	rVV3	2308	2834	0.40%	0.034%
24	14.316	1854	1860	1867	rVB	255458	354089	50.50%	4.297%
25	14.628	1906	1913	1919	rBV	293560	464329	66.22%	5.635%
26	14.839	1946	1949	1952	rBV3	2842	3391	0.48%	0.041%
27	14.921	1956	1963	1971	rBV	227690	358740	51.16%	4.353%
28	15.092	1983	1992	2002	rBV	67649	113201	16.14%	1.374%
29	15.632	2079	2084	2089	rBV2	3890	7446	1.06%	0.090%
30	15.909	2125	2131	2138	rVB	368889	572926	81.71%	6.952%
31	16.014	2144	2149	2155	rVB	103111	146198	20.85%	1.774%
32	16.097	2159	2163	2166	rBV	1624	2204	0.31%	0.027%
33	16.449	2220	2223	2226	rVB3	2569	2447	0.35%	0.030%
34	16.537	2237	2238	2243	rVB2	2714	2809	0.40%	0.034%
35	16.602	2245	2249	2252	rBV	2247	2446	0.35%	0.030%
36	16.760	2272	2276	2281	rVB2	11188	13668	1.95%	0.166%

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37	17.001	2313	2317	2321	rVB3	1717	2622	0.37%	0.032%
38	17.119	2331	2337	2339	rBV	2184	3615	0.52%	0.044%
39	17.348	2369	2376	2377	rBV3	3213	5244	0.75%	0.064%
40	17.366	2377	2379	2382	rVB	2712	3016	0.43%	0.037%

41	17.389	2382	2383	2387	rBV	2105	2555	0.36%	0.031%
42	17.507	2398	2403	2405	rBV4	2653	4205	0.60%	0.051%
43	17.671	2424	2431	2440	rBV	290737	447222	63.78%	5.427%
44	17.771	2442	2448	2456	rBV	431671	626174	89.30%	7.599%
45	18.129	2505	2509	2510	rBV	2015	2362	0.34%	0.029%

46	18.270	2528	2533	2539	rVB4	2814	5226	0.75%	0.063%
47	18.364	2545	2549	2550	rBV2	3019	3969	0.57%	0.048%
48	18.435	2556	2561	2565	rBV2	13406	20578	2.93%	0.250%
49	18.488	2566	2570	2583	rVB2	78726	122194	17.43%	1.483%
50	18.899	2635	2640	2642	rBV5	2500	3841	0.55%	0.047%

51	19.158	2681	2684	2686	rBV3	2782	2930	0.42%	0.036%
52	19.281	2701	2705	2707	rVB3	2136	2497	0.36%	0.030%
53	19.387	2721	2723	2727	rVB3	4380	4009	0.57%	0.049%
54	19.434	2727	2731	2737	rVB3	39332	47989	6.84%	0.582%
55	19.616	2758	2762	2765	rBV5	8453	14346	2.05%	0.174%

56	19.751	2781	2785	2792	rBV2	14326	20890	2.98%	0.253%
57	19.810	2794	2795	2798	rVB3	3331	2500	0.36%	0.030%
58	19.839	2798	2800	2807	rVB4	2162	2910	0.42%	0.035%
59	19.898	2807	2810	2811	rBV2	3311	2906	0.41%	0.035%
60	19.933	2814	2816	2818	rBV2	2913	2728	0.39%	0.033%

61	20.010	2827	2829	2830	rBV2	5077	4604	0.66%	0.056%
62	20.045	2830	2835	2843	rVB	477938	677446	96.61%	8.221%
63	20.280	2872	2875	2880	rVB6	3402	3553	0.51%	0.043%
64	20.391	2890	2894	2896	rBV2	2695	3659	0.52%	0.044%
65	20.480	2904	2909	2910	rBV4	5292	7479	1.07%	0.091%

66	20.697	2936	2946	2948	rBV5	4390	8817	1.26%	0.107%
67	21.126	3016	3019	3024	rBV7	3465	5769	0.82%	0.070%
68	21.226	3032	3036	3041	rVB7	7859	10018	1.43%	0.122%
69	21.537	3084	3089	3102	rBV2	56589	102092	14.56%	1.239%
70	21.661	3106	3110	3117	rVB6	9703	16004	2.28%	0.194%

71	21.919	3152	3154	3155	rVV2	3228	2388	0.34%	0.029%
72	21.937	3155	3157	3158	rVV2	4364	2556	0.36%	0.031%
73	21.990	3159	3166	3174	rVB2	235876	430589	61.41%	5.225%
74	22.524	3253	3257	3262	rBV5	8676	14475	2.06%	0.176%
75	22.624	3270	3274	3282	rVB7	13124	26238	3.74%	0.318%

76	22.759	3294	3297	3298	rBV3	5887	5954	0.85%	0.072%
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77	22.806	3302	3305	3307	rBV4	4822	6871	0.98%	0.083%
78	23.253	3379	3381	3384	rVB4	2659	2513	0.36%	0.030%
79	23.511	3419	3425	3426	rBV5	7150	11495	1.64%	0.139%
80	23.717	3457	3460	3467	rVB6	8279	15441	2.20%	0.187%
81	24.399	3568	3576	3583	rBV3	45653	102791	14.66%	1.247%
82	25.074	3689	3691	3693	rVB2	2891	2256	0.32%	0.027%
83	25.286	3715	3727	3741	rBV3	224695	701203	100.00%	8.509%
84	25.533	3760	3769	3782	rVB2	162508	479390	68.37%	5.817%
85	25.838	3819	3821	3823	rBV3	2875	2164	0.31%	0.026%
86	25.903	3828	3832	3834	rBV4	3653	5036	0.72%	0.061%
87	26.108	3865	3867	3870	rBV4	2427	2720	0.39%	0.033%
88	26.690	3960	3966	3975	rVB5	18277	51131	7.29%	0.620%
89	27.207	4051	4054	4055	rBV3	3273	3678	0.52%	0.045%
90	28.035	4193	4195	4197	rBV3	2536	2241	0.32%	0.027%
91	28.188	4219	4221	4222	rBV2	4303	4277	0.61%	0.052%
92	28.323	4242	4244	4249	rVB6	2886	4474	0.64%	0.054%
93	29.645	4467	4469	4471	rBV3	3436	2586	0.37%	0.031%
94	30.292	4578	4579	4584	rBV4	2852	4347	0.62%	0.053%
95	30.797	4661	4665	4666	rBV3	3049	3582	0.51%	0.043%
96	30.832	4669	4671	4673	rBV2	2514	2237	0.32%	0.027%
97	31.326	4748	4755	4756	rBV4	5839	11946	1.70%	0.145%
98	31.561	4794	4795	4797	rBV2	3838	3043	0.43%	0.037%
99	32.189	4900	4902	4904	rBV3	2560	2222	0.32%	0.027%
100	32.242	4909	4911	4913	rVV2	3263	2824	0.40%	0.034%

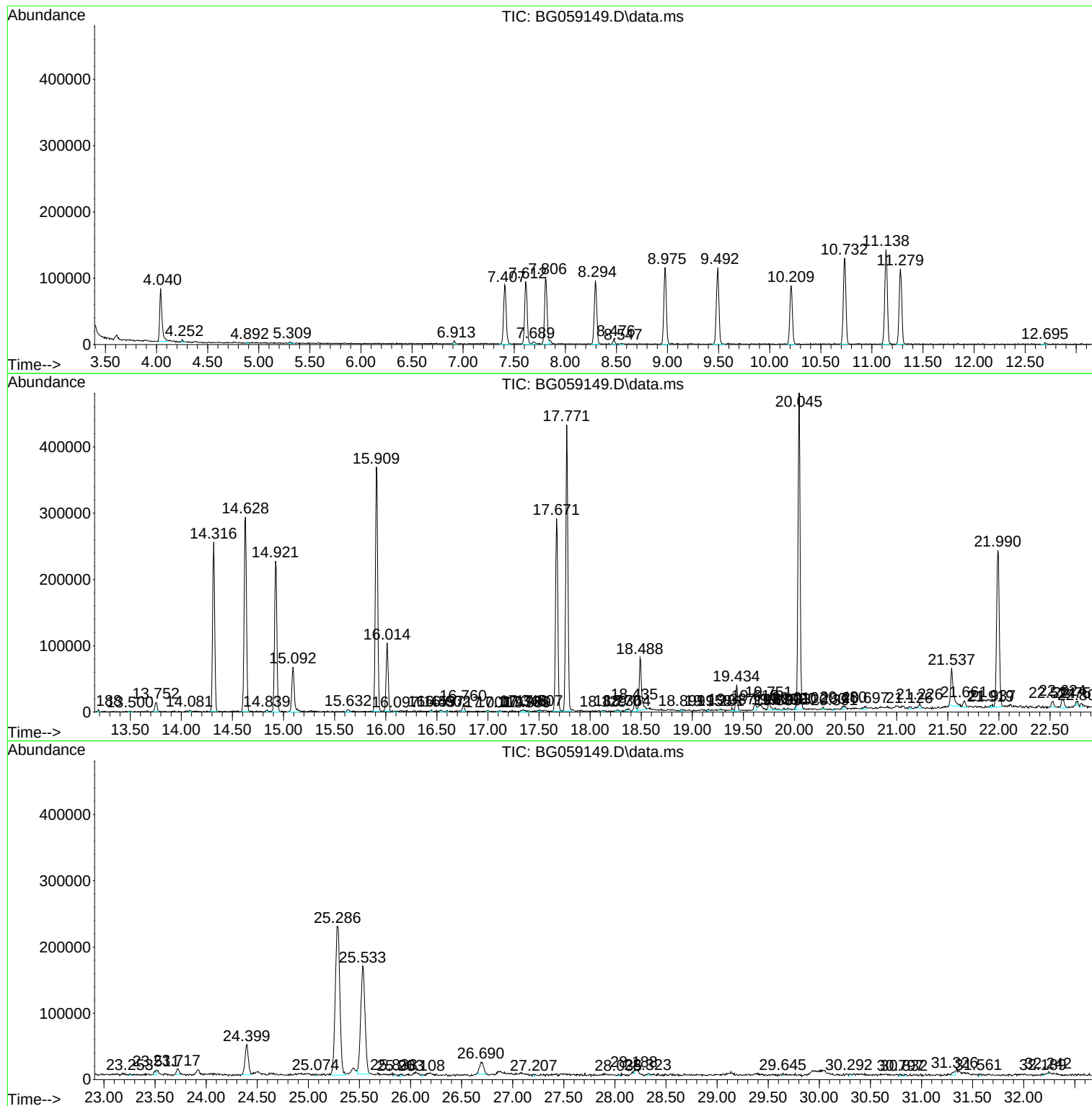
Sum of corrected areas: 8240729

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091923.MA.M
Quant Title : SVOA CALIBRATION

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



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Instrument :
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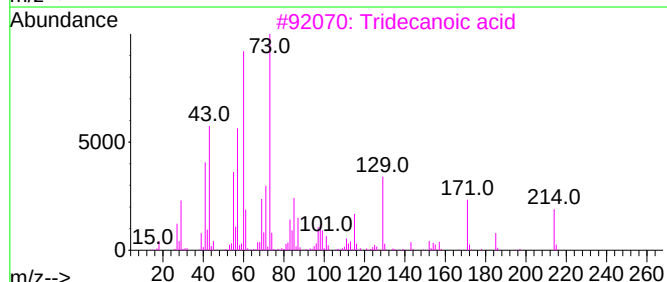
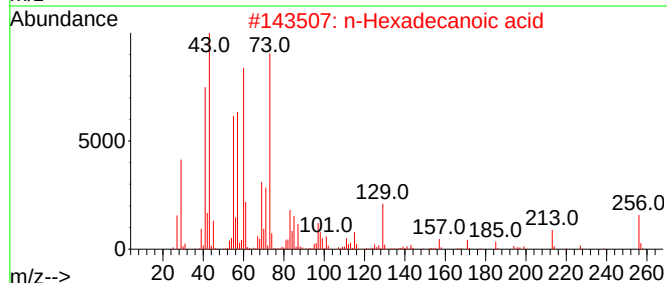
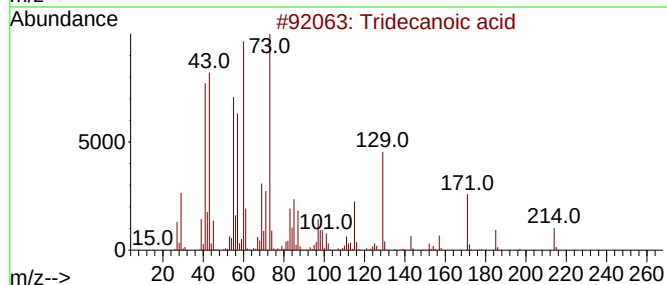
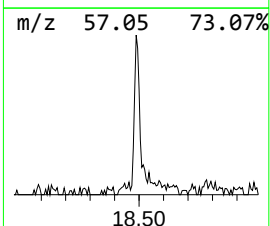
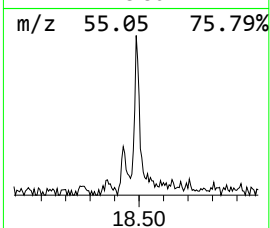
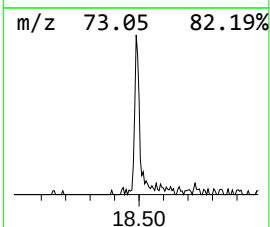
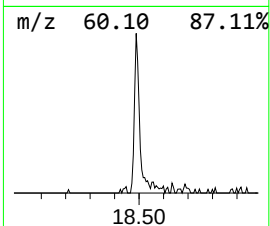
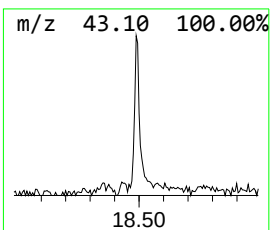
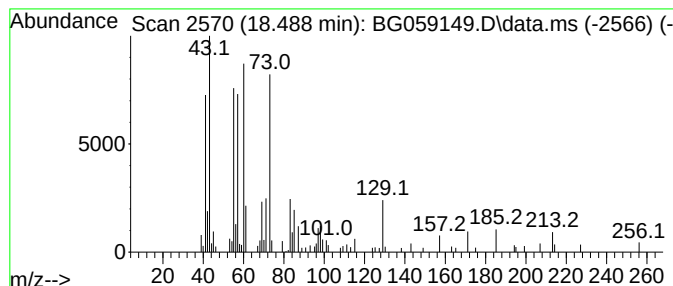
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091923.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Tridecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.488	5.46 ng/ul	122194	Phenanthrene-d10	17.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	72



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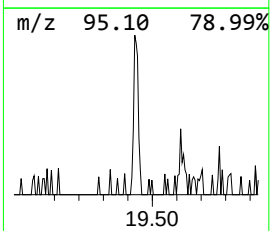
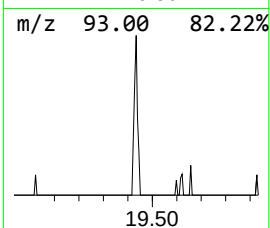
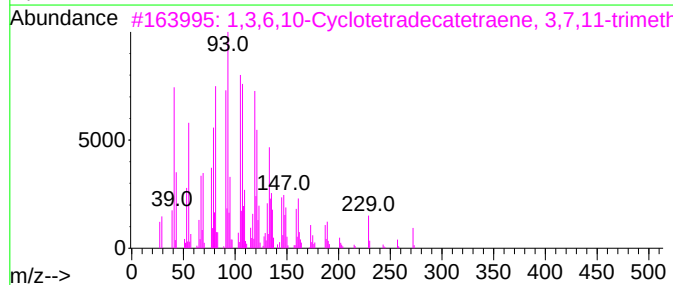
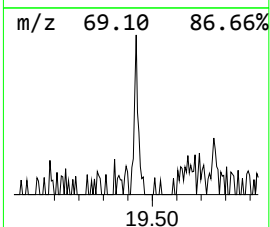
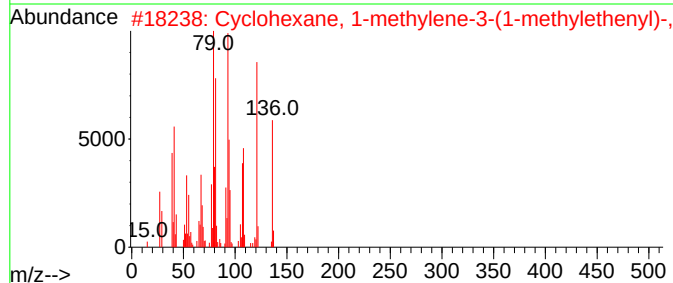
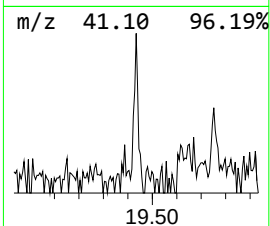
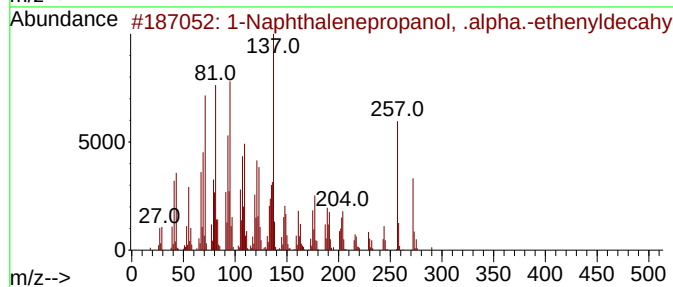
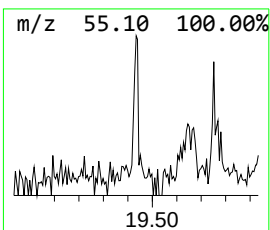
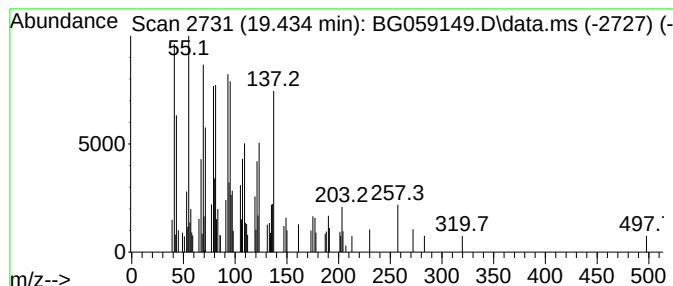
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091923.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
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Peak Number 2 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.434	2.15 ng/ul	47989	Phenanthrene-d10	17.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenepropanol, .alpha.-e...	290	C20H34O	000596-85-0	49		
2	Cyclohexane, 1-methylene-3-(1-me...	136	C10H16	013837-95-1	46		
3	1,3,6,10-Cyclotetradecatetraene,...	272	C20H32	001898-13-1	38		
4	1,1,6-trimethyl-3-methylene-2-(3...	452	C33H56	1000373-94-5	38		
5	Acetic acid, 3-(5,5-dimethyl-spi...	250	C16H26O2	077143-33-0	35		



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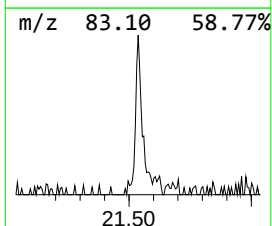
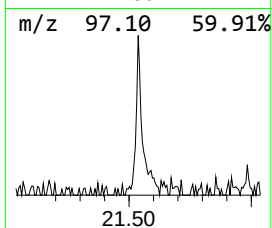
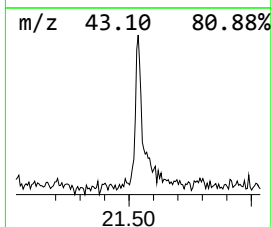
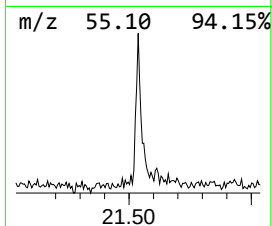
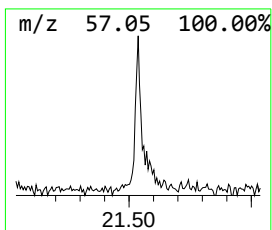
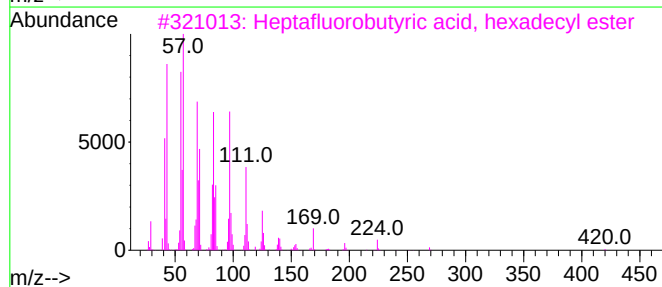
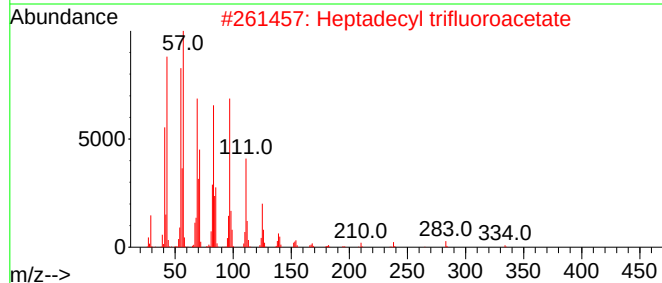
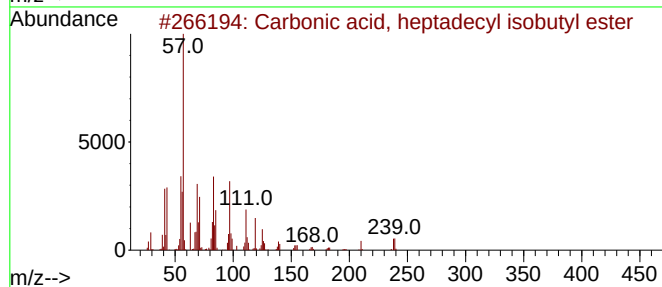
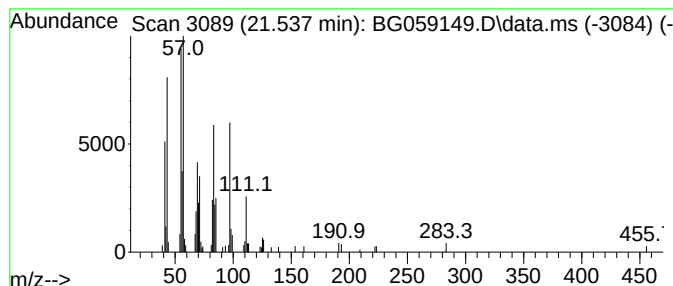
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TIC Library : C:\DATABASE\NIST20.L
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Peak Number 3 Carbonic acid, heptadecyl i... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.537	4.74 ng/ul	102092	Chrysene-d12	21.990

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	91
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	86
4			1-Octadecanol	270	C18H38O	000112-92-5	86
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092023\
Data File : BG059149.D
Acq On : 21 Sep 2023 21:27
Operator : MA/JU
Sample : 04386-06
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AB9

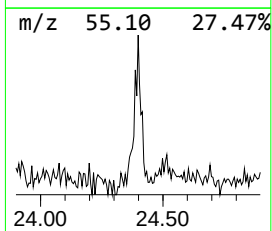
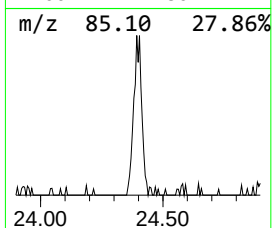
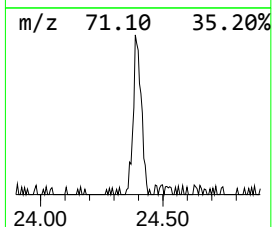
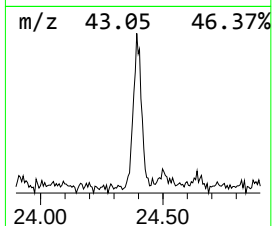
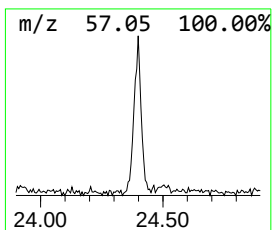
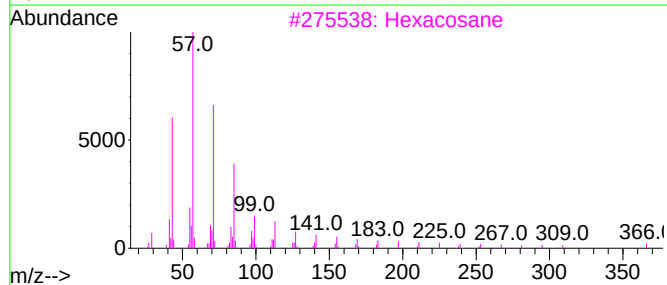
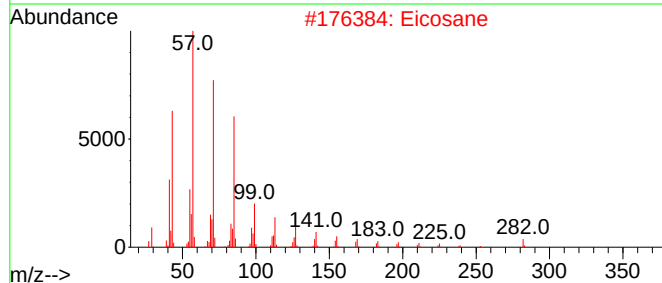
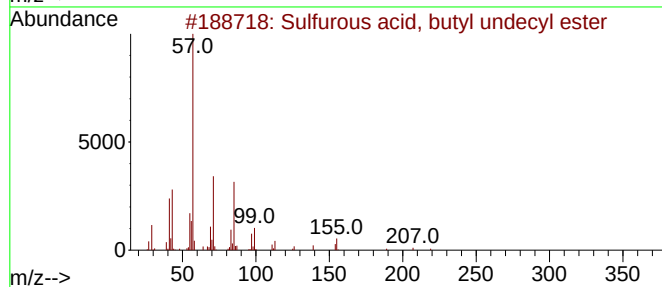
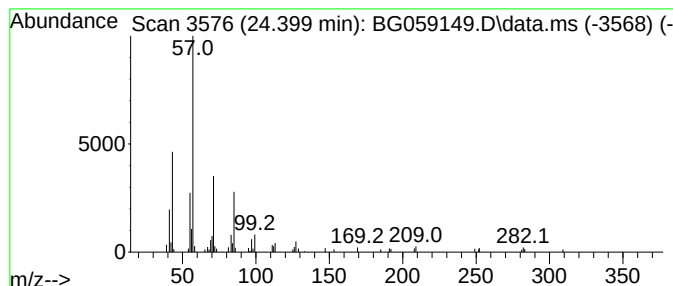
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Sulfurous acid, butyl undec... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.399	4.29 ng/ul	102791	Perylene-d12	25.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	64
2			Eicosane	282	C20H42	000112-95-8	64
3			Hexacosane	366	C26H54	000630-01-3	53
4			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	50
5			Pentacosane	352	C25H52	000629-99-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092023\
Data File : BG059149.D
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Operator : MA/JU
Sample : 04386-06
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AB9

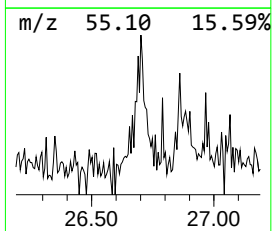
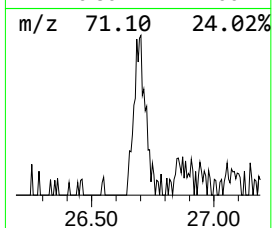
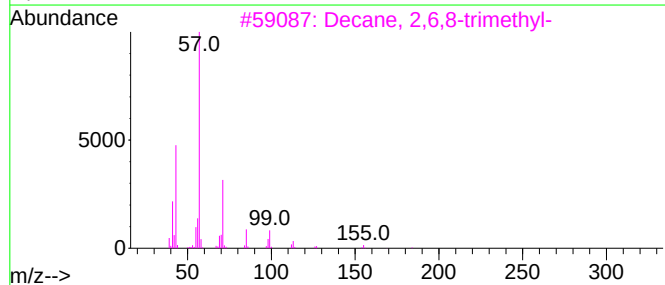
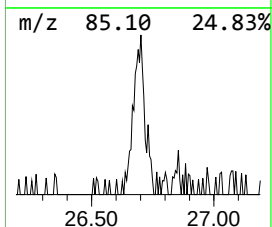
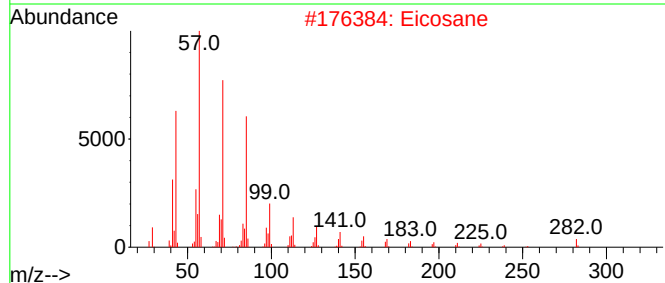
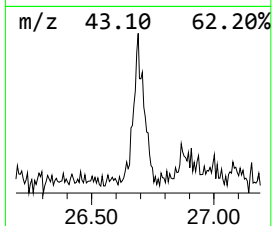
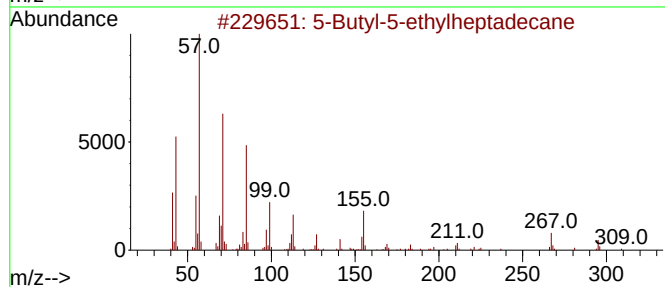
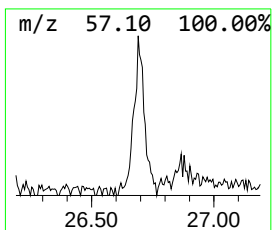
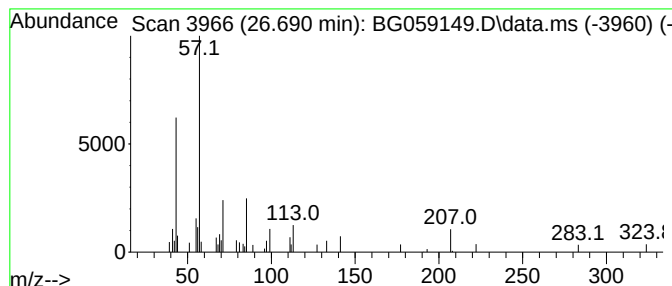
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.690	2.13 ng/ul	51131	Perylene-d12	25.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Butyl-5-ethylheptadecane	324	C23H48	1000360-43-0	50
2			Eicosane	282	C20H42	000112-95-8	43
3			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	38
4			Tricosane	324	C23H48	000638-67-5	38
5			Tridecane, 7-propyl-	226	C16H34	055045-09-5	38



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Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AB9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091923.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
Tridecanoic acid	18.488	5.5	ng/ul	122194	4	17.671	447222	20.0
unknown-01	19.434	2.1	ng/ul	47989	4	17.671	447222	20.0
Carbonic acid, ...	21.537	4.7	ng/ul	102092	5	21.990	430589	20.0
Sulfurous acid,...	24.399	4.3	ng/ul	102791	6	25.532	479390	20.0
(DEL) Alkane: S...	26.690	2.1	ng/ul	51131	6	25.532	479390	20.0