

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
 Data File : BG062319.D
 Acq On : 8 Aug 2024 4:30
 Operator : MA/JU
 Sample : P3437-05
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :

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: BG062319.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.423	19	23	29	rVB	12407	15890	0.69%	0.065%
2	3.681	64	67	72	rBV2	7289	10478	0.45%	0.043%
3	3.828	87	92	102	rBV	47866	82111	3.54%	0.338%
4	4.163	146	149	153	rBV3	2919	4005	0.17%	0.016%
5	4.380	182	186	192	rVB4	3833	6362	0.27%	0.026%
6	6.042	465	469	474	rBV2	3275	5514	0.24%	0.023%
7	7.112	644	651	659	rBV	91860	159165	6.87%	0.655%
8	7.288	672	681	693	rBV	193623	326986	14.12%	1.346%
9	7.488	708	715	723	rBV	239630	404970	17.48%	1.668%
10	7.958	788	795	802	rBV	246071	409236	17.67%	1.685%
11	8.022	802	806	813	rVB4	3612	5708	0.25%	0.024%
12	8.651	906	913	921	rBV	236881	403143	17.40%	1.660%
13	9.109	983	991	999	rBV	257352	446119	19.26%	1.837%
14	9.215	1004	1009	1016	rVV3	2790	5188	0.22%	0.021%
15	9.673	1078	1087	1092	rBV	17943	27875	1.20%	0.115%
16	9.826	1106	1113	1123	rBV	206454	367532	15.87%	1.513%
17	9.967	1130	1137	1145	rBV	17492	37447	1.62%	0.154%
18	10.366	1196	1205	1214	rBV	378746	665678	28.74%	2.741%
19	10.748	1263	1270	1279	rVB	367625	662176	28.59%	2.727%
20	10.877	1283	1292	1304	rBV	193760	352913	15.24%	1.453%
21	11.282	1354	1361	1365	rVV2	5899	8947	0.39%	0.037%
22	11.482	1388	1395	1402	rBV	34315	61491	2.65%	0.253%
23	12.334	1532	1540	1544	rBV2	6618	10676	0.46%	0.044%
24	13.203	1682	1688	1694	rBV	8568	12050	0.52%	0.050%
25	13.421	1718	1725	1727	rBV3	2244	3940	0.17%	0.016%
26	13.985	1813	1821	1827	rBV	726612	1055749	45.58%	4.347%
27	14.267	1855	1869	1878	rBV	782082	1250346	53.98%	5.149%
28	14.349	1880	1883	1890	rBV5	3728	7173	0.31%	0.030%
29	14.578	1914	1922	1928	rVV	690640	1088125	46.97%	4.481%
30	14.678	1933	1939	1944	rVB2	48695	66862	2.89%	0.275%
31	14.748	1944	1951	1956	rBV	106304	172134	7.43%	0.709%
32	14.913	1974	1979	1983	rVB7	4899	7119	0.31%	0.029%
33	14.983	1987	1991	1996	rBV5	6509	10458	0.45%	0.043%
34	15.312	2043	2047	2053	rVB	62169	85306	3.68%	0.351%
35	15.383	2056	2059	2065	rBV6	2990	5533	0.24%	0.023%
36	15.565	2083	2090	2102	rBV	1061456	1638095	70.72%	6.746%

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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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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
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37	15.671	2102	2108	2118	rBV	288092	418819	18.08%	1.725%
38	15.741	2118	2120	2124	rVV5	2826	3373	0.15%	0.014%
39	15.806	2127	2131	2134	rVV5	3783	5582	0.24%	0.023%
40	16.235	2197	2204	2209	rBV2	31519	46247	2.00%	0.190%
41	16.299	2211	2215	2218	rVV4	6027	8454	0.36%	0.035%
42	16.722	2283	2287	2292	rBV6	8308	13943	0.60%	0.057%
43	16.875	2309	2313	2315	rBV5	3603	5278	0.23%	0.022%
44	16.928	2320	2322	2327	rVB6	2455	3660	0.16%	0.015%
45	16.986	2328	2332	2336	rVB5	5572	8167	0.35%	0.034%
46	17.057	2339	2344	2347	rBV7	5439	11851	0.51%	0.049%
47	17.098	2348	2351	2355	rVB5	4864	6567	0.28%	0.027%
48	17.245	2374	2376	2381	rBV6	6508	6066	0.26%	0.025%
49	17.315	2381	2388	2395	rBV	836230	1272242	54.92%	5.239%
50	17.415	2398	2405	2412	rVB2	1134127	1786025	77.10%	7.355%
51	17.492	2415	2418	2419	rBV2	5199	5339	0.23%	0.022%
52	17.668	2446	2448	2451	rBV4	4104	6024	0.26%	0.025%
53	17.703	2451	2454	2458	rVB7	5218	9073	0.39%	0.037%
54	17.938	2490	2494	2499	rBV8	7589	12426	0.54%	0.051%
55	17.991	2500	2503	2508	rVB6	7176	11676	0.50%	0.048%
56	18.085	2516	2519	2522	rBV5	4413	5944	0.26%	0.024%
57	18.220	2536	2542	2550	rBV	304746	454574	19.62%	1.872%
58	18.520	2591	2593	2599	rBV6	5100	7252	0.31%	0.030%
59	18.684	2617	2621	2625	rVB7	6275	10669	0.46%	0.044%
60	18.884	2651	2655	2659	rBV7	7371	11847	0.51%	0.049%
61	19.019	2672	2678	2683	rBV	116830	169439	7.31%	0.698%
62	19.066	2683	2686	2697	rVV	21981	56617	2.44%	0.233%
63	19.148	2698	2700	2705	rVB5	9783	12381	0.53%	0.051%
64	19.260	2716	2719	2723	rVB	17865	22365	0.97%	0.092%
65	19.330	2726	2731	2735	rBV2	25327	38815	1.68%	0.160%
66	19.366	2735	2737	2742	rVB6	9572	10333	0.45%	0.043%
67	19.489	2753	2758	2766	rBV	144635	217559	9.39%	0.896%
68	19.642	2780	2784	2786	rBV5	7694	10312	0.45%	0.042%
69	19.695	2786	2793	2801	rVV	1551014	2207363	95.29%	9.090%
70	20.041	2850	2852	2855	rBV3	4522	5039	0.22%	0.021%
71	20.118	2861	2865	2869	rVB4	28907	36499	1.58%	0.150%
72	20.217	2878	2882	2886	rBV4	20579	26340	1.14%	0.108%
73	20.253	2886	2888	2892	rVB3	13704	13512	0.58%	0.056%
74	20.576	2939	2943	2946	rVV5	11044	16069	0.69%	0.066%
75	20.699	2962	2964	2968	rBV4	11465	12992	0.56%	0.053%
76	21.234	3051	3055	3062	rBV2	106824	165343	7.14%	0.681%

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Peak Location: TOP

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77	21.551	3103	3109	3118	rBV	850817	1411124	60.92%	5.811%
78	21.780	3145	3148	3154	rBV8	9612	13719	0.59%	0.056%
79	22.174	3213	3215	3219	rVB5	8066	9101	0.39%	0.037%
80	22.238	3222	3226	3232	rVB8	23780	42304	1.83%	0.174%
81	22.344	3240	3244	3248	rBV4	27144	48203	2.08%	0.198%
82	22.526	3266	3275	3287	rVB6	55461	161780	6.98%	0.666%
83	22.661	3293	3298	3303	rBV4	38244	69676	3.01%	0.287%
84	22.720	3303	3308	3318	rVB3	106969	212012	9.15%	0.873%
85	22.920	3338	3342	3346	rBV3	28027	51961	2.24%	0.214%
86	23.231	3387	3395	3403	rBV	351006	667223	28.80%	2.748%
87	23.824	3492	3496	3503	rBV3	20039	38460	1.66%	0.158%
88	24.435	3589	3600	3612	rVB	879318	2316411	100.00%	9.539%
89	24.641	3624	3635	3647	rBV	543829	1532035	66.14%	6.309%
90	24.741	3647	3652	3660	rVB5	16822	40463	1.75%	0.167%
91	24.858	3670	3672	3675	rBV4	4000	3830	0.17%	0.016%
92	25.845	3834	3840	3845	rVB4	13403	32136	1.39%	0.132%
93	25.933	3850	3855	3856	rBV5	18529	25840	1.12%	0.106%
94	26.791	3992	4001	4008	rBV5	19794	59076	2.55%	0.243%
95	26.967	4025	4031	4042	rVB5	10532	34665	1.50%	0.143%
96	27.149	4056	4062	4070	rVB8	11804	31960	1.38%	0.132%
97	28.718	4318	4329	4338	rBV8	26824	106330	4.59%	0.438%
98	28.947	4357	4368	4379	rVB8	31979	135000	5.83%	0.556%
99	29.564	4471	4473	4475	rBV3	3954	3712	0.16%	0.015%
100	30.039	4543	4554	4568	rVB3	43638	202639	8.75%	0.834%

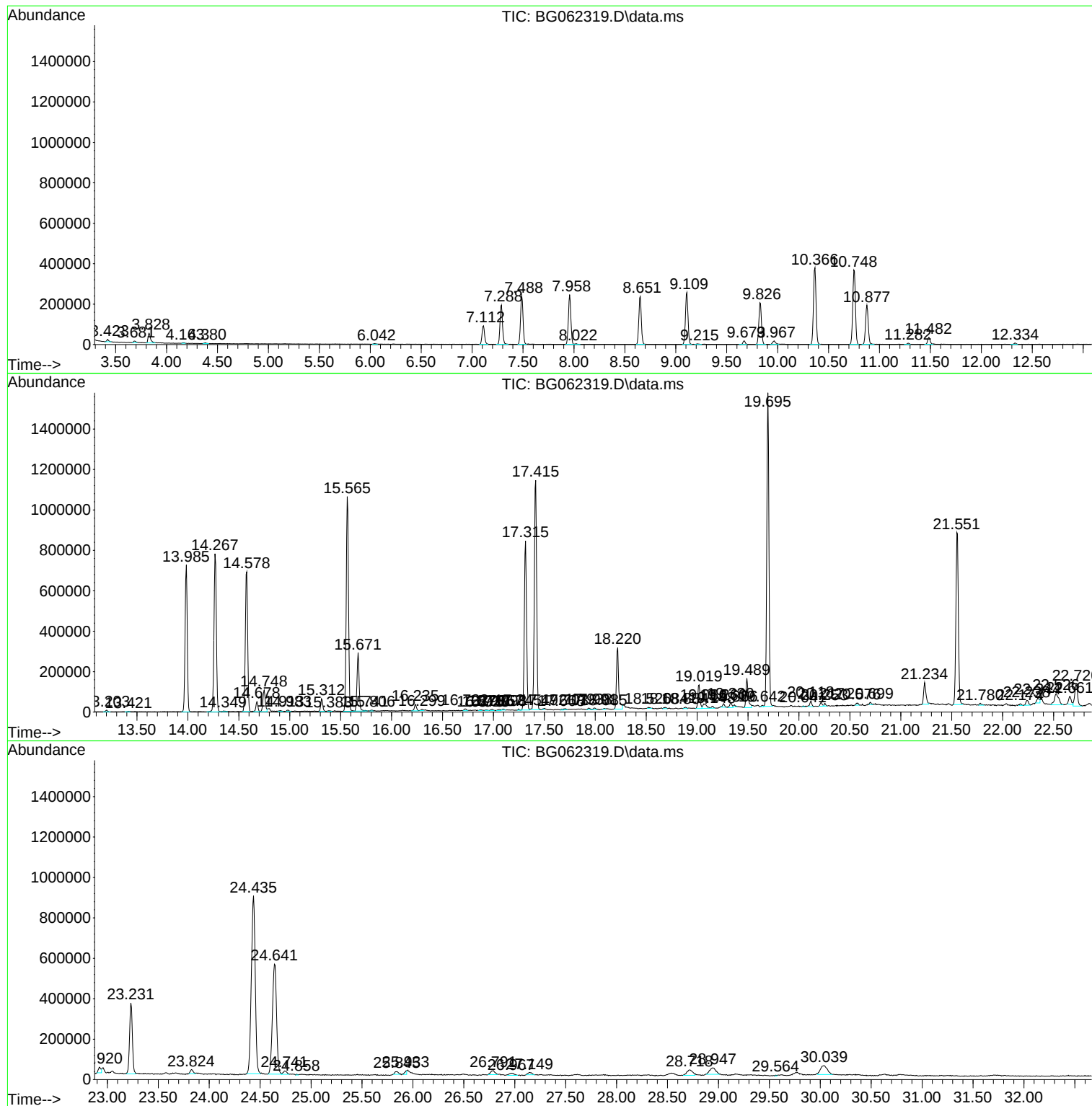
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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



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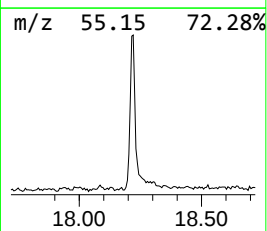
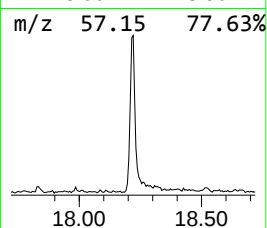
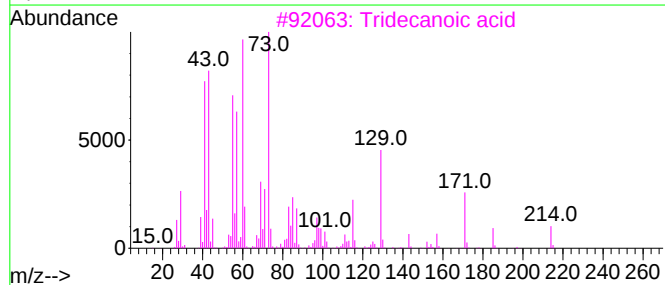
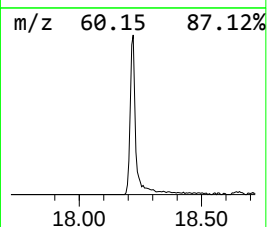
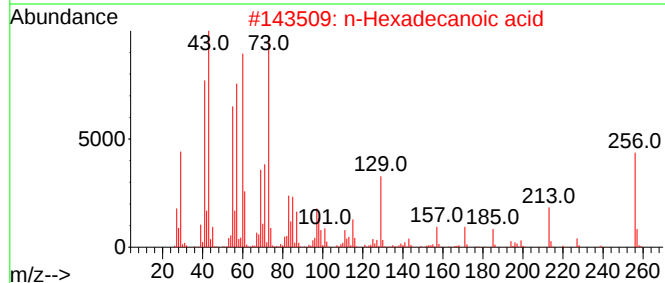
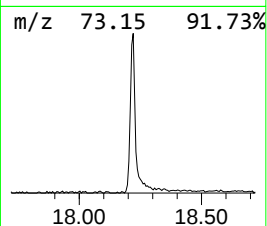
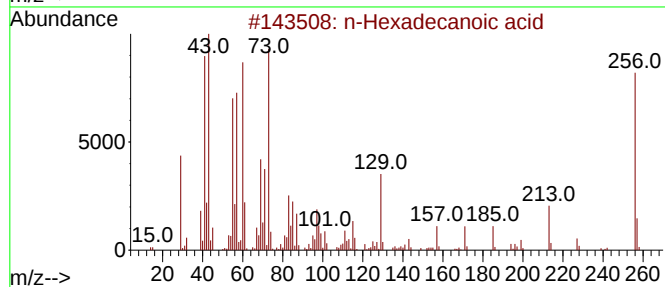
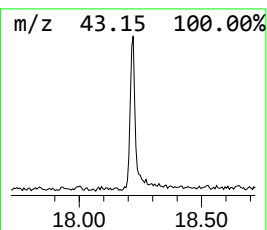
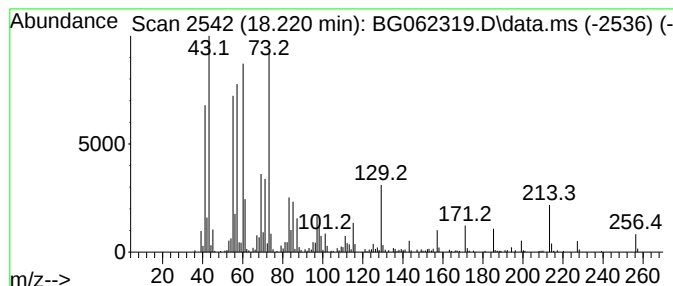
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.220	7.15 ng/ul	454574	Phenanthrene-d10	17.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	95
4			Tridecanoic acid	214	C13H26O2	000638-53-9	94
5			Tridecanoic acid	214	C13H26O2	000638-53-9	93



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Misc :
ALS Vial : 24 Sample Multiplier: 1

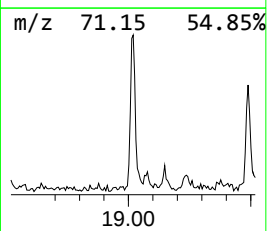
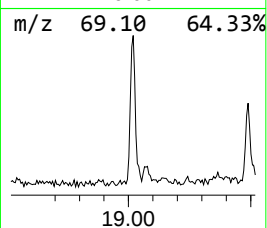
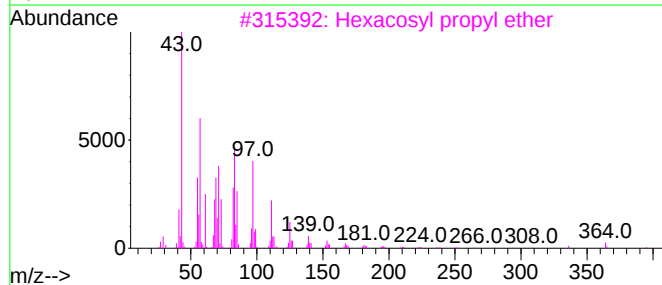
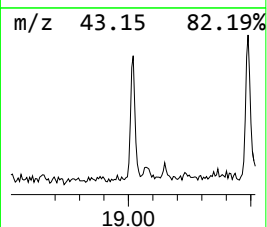
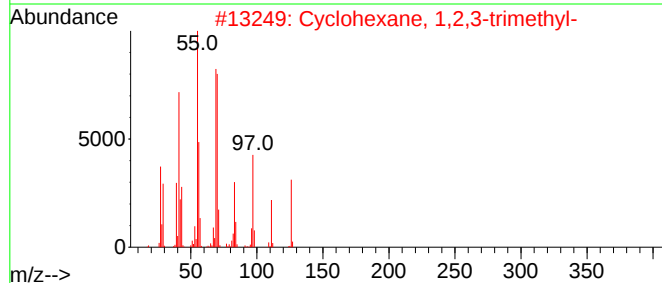
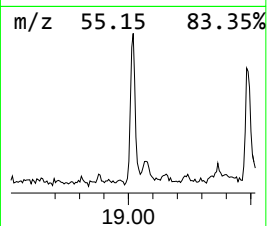
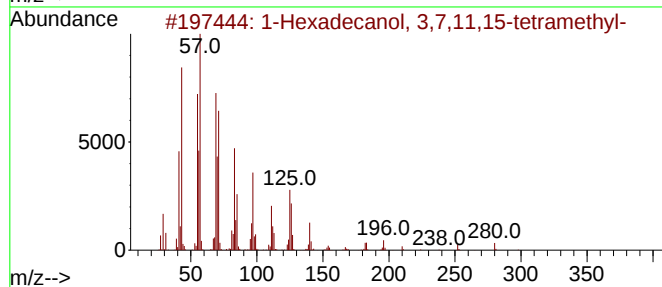
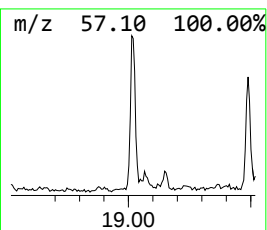
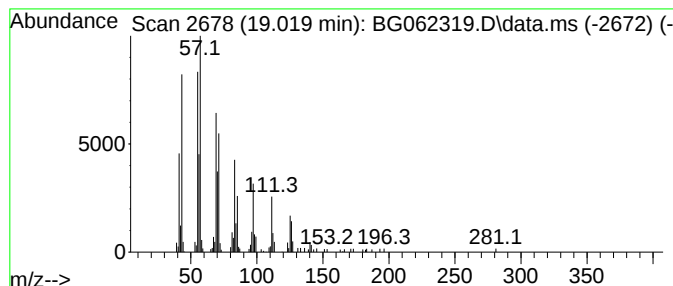
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 1-Hexadecanol, 3,7,11,15-te... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.019	2.66 ng/ul	169439	Phenanthrene-d10	17.316	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol, 3,7,11,15-tetrame...	298	C20H42O	000645-72-7	86
2	Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	60
3	Hexacosyl propyl ether	424	C29H60O	1000406-28-4	52
4	Propyl triacontyl ether	481	C33H68O	1000406-28-6	52
5	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	52



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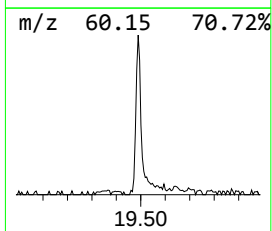
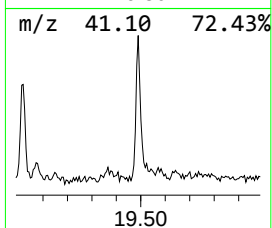
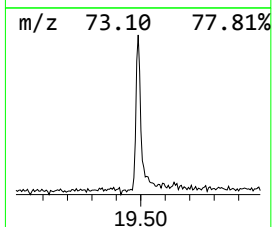
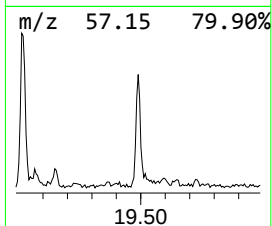
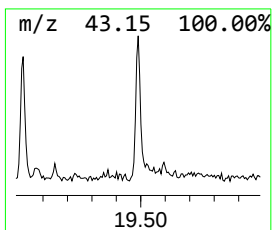
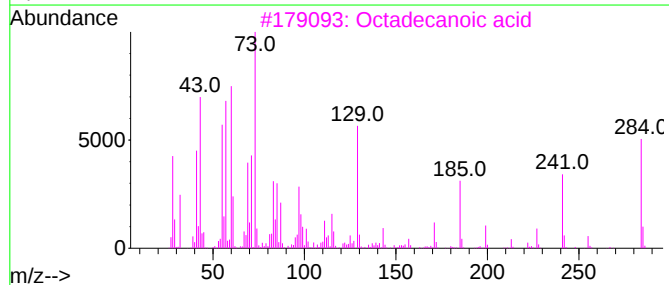
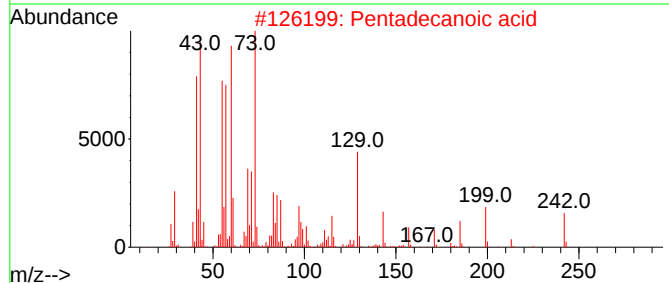
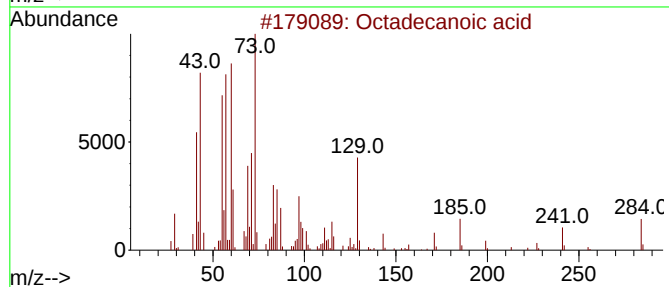
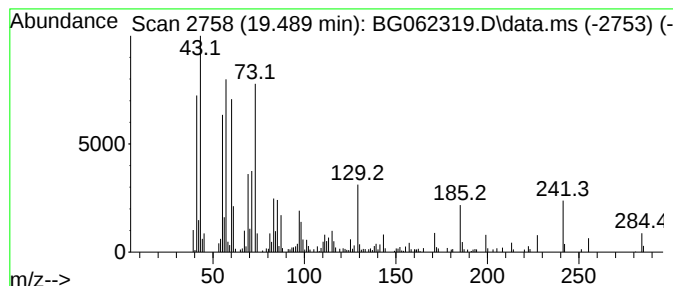
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.489	3.08 ng/ul	217559	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Octadecanoic acid	284	C18H36O2	000057-11-4	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Octadecanoic acid	284	C18H36O2	000057-11-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062319.D
Acq On : 8 Aug 2024 4:30
Operator : MA/JU
Sample : P3437-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

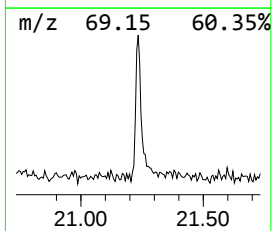
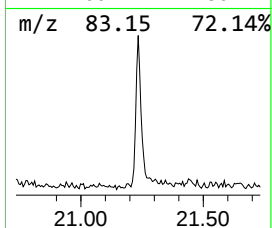
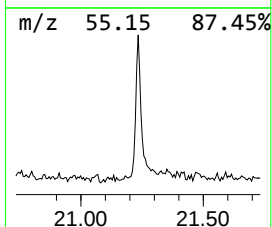
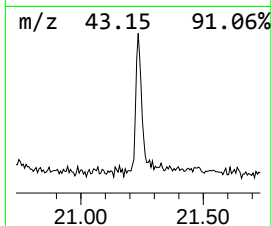
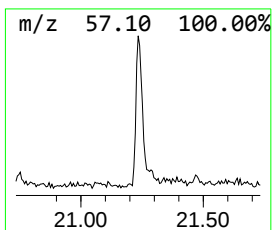
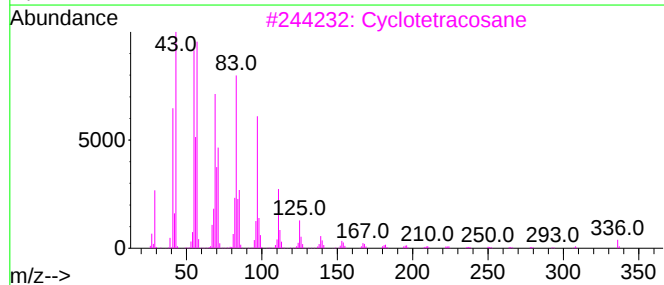
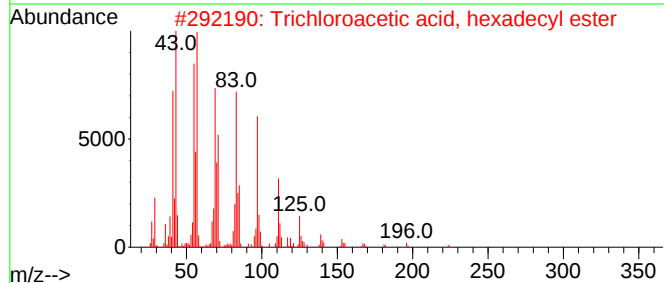
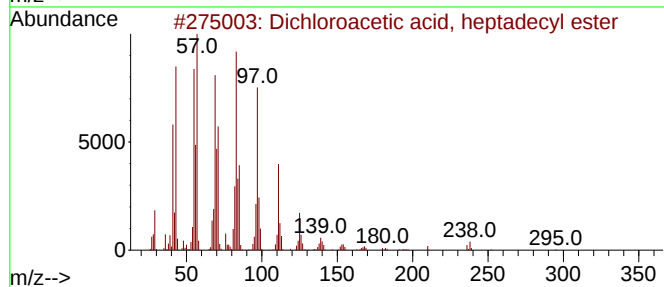
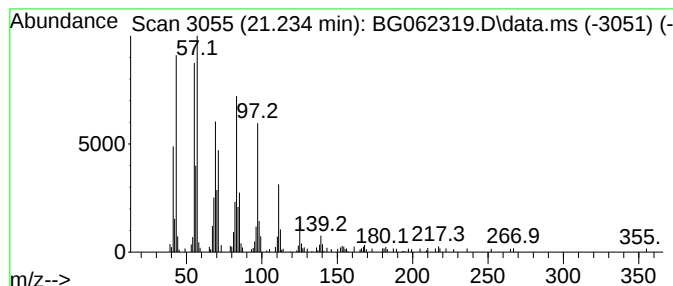
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ClientSampleId :

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 4 Dichloroacetic acid, heptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.234	2.34 ng/ul	165343	Chrysene-d12	21.551	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
3	Cyclotetracosane	336	C24H48	000297-03-0	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5	1-Hexacosene	364	C26H52	018835-33-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062319.D
Acq On : 8 Aug 2024 4:30
Operator : MA/JU
Sample : P3437-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

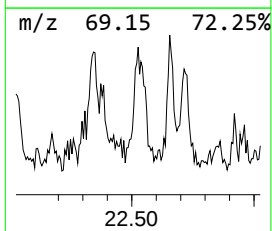
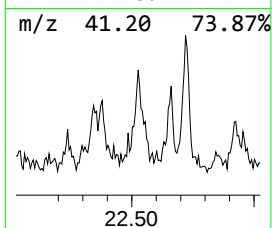
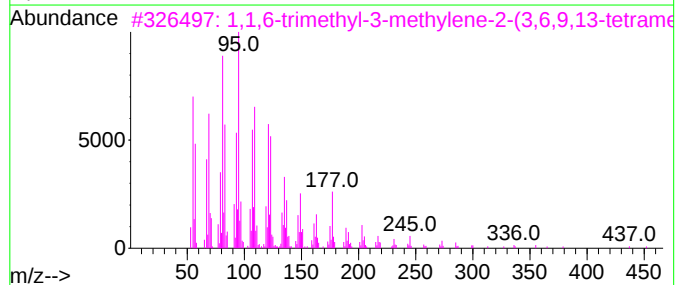
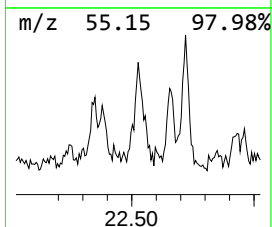
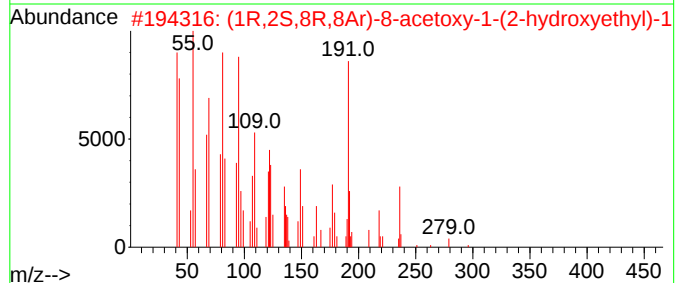
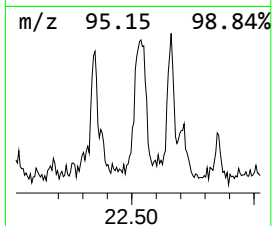
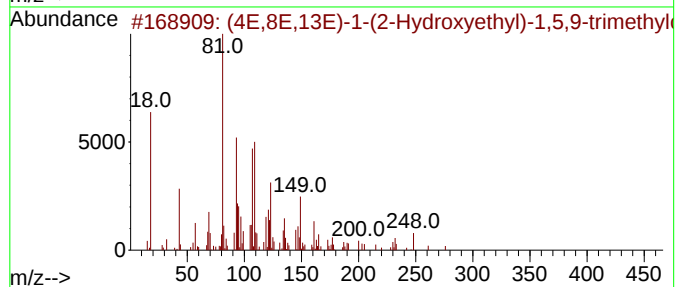
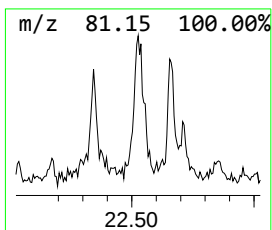
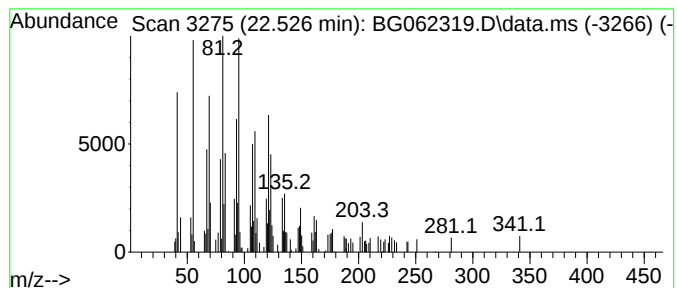
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (4E,8E,13E)-1-(2-Hydroxyeth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.526	2.29 ng/ul	161780	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(4E,8E,13E)-1-(2-Hydroxyethyl)-1...	276	C19H32O	1000426-96-0	58
2			(1R,2S,8R,8Ar)-8-acetoxy-1-(2-hy...	296	C18H32O3	1000298-98-4	58
3			1,1,6-trimethyl-3-methylene-2-(3...	452	C33H56	1000373-94-5	58
4			trans-Geranylgeraniol	290	C20H34O	024034-73-9	43
5			Isolongifolol	222	C15H26O	001139-17-9	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062319.D
Acq On : 8 Aug 2024 4:30
Operator : MA/JU
Sample : P3437-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :

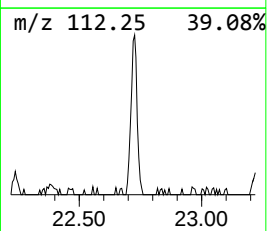
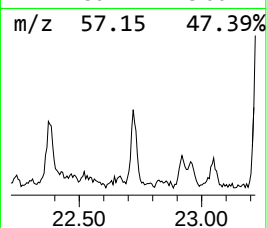
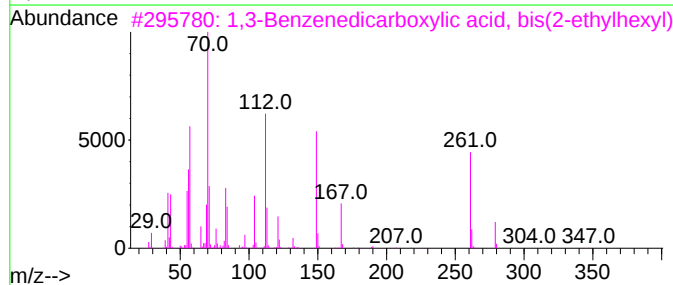
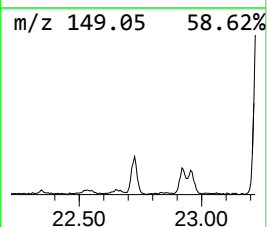
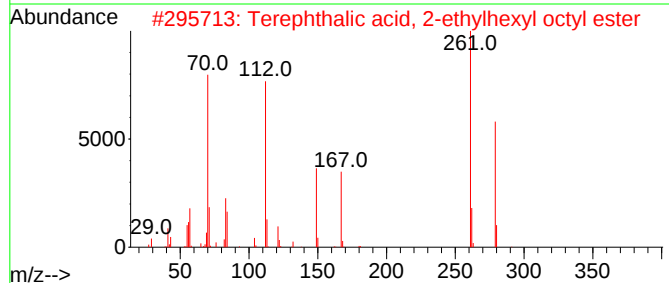
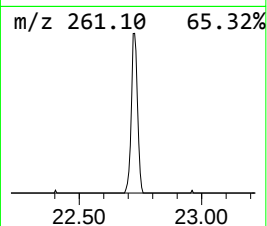
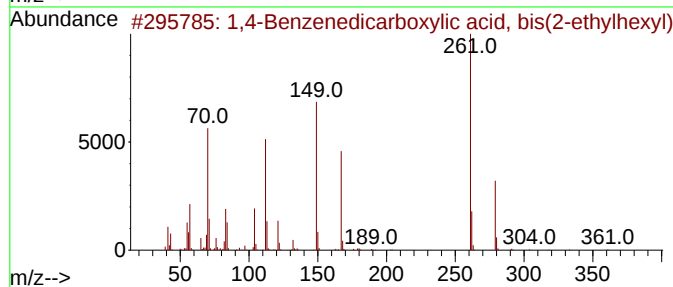
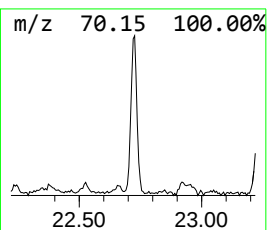
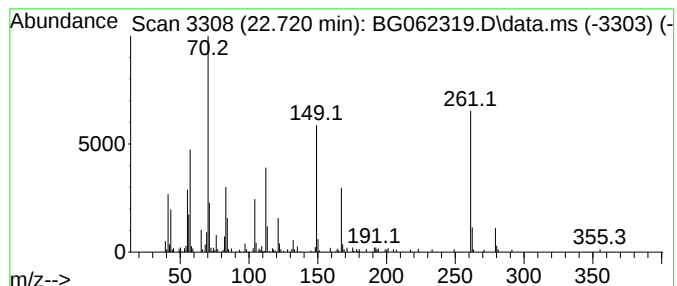
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.720	3.00 ng/ul	212012	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
2			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	58
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	53
4			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
5			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062319.D
Acq On : 8 Aug 2024 4:30
Operator : MA/JU
Sample : P3437-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

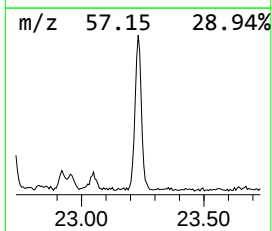
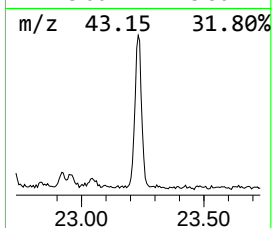
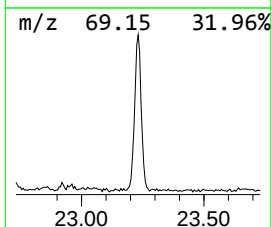
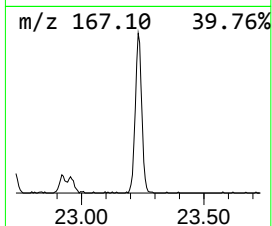
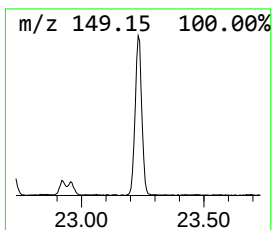
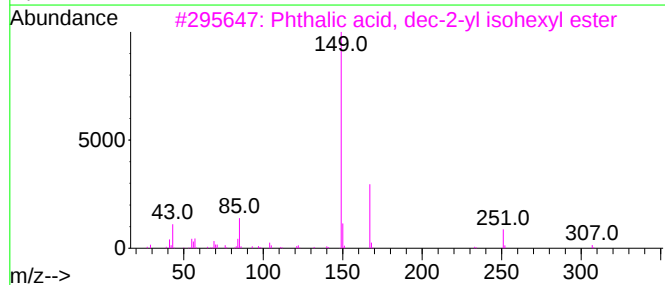
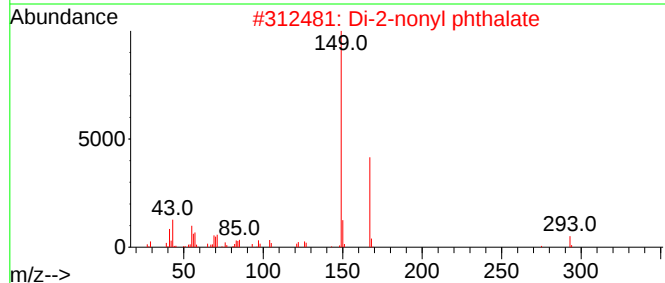
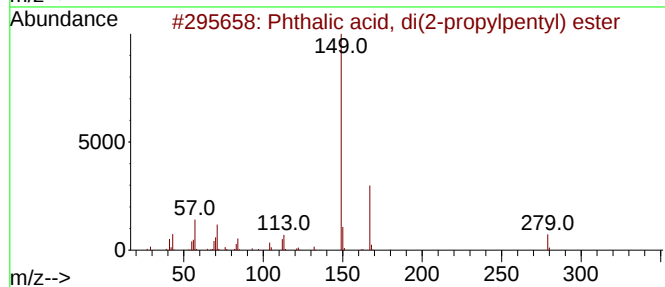
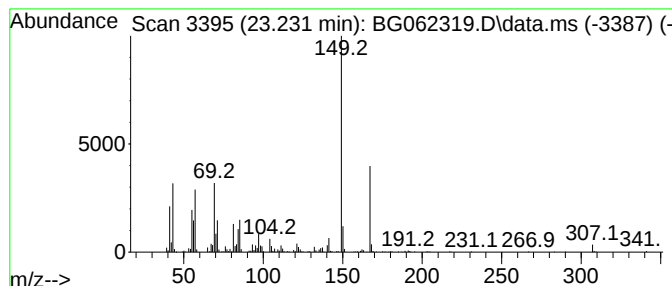
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Phthalic acid, di(2-propylp... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.231	8.71 ng/ul	667223	Perylene-d12	24.641

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, di(2-propylpentyl...)	390	C24H38O4	1000377-93-5	72
2			Di-2-nonyl phthalate	418	C26H42O4	059431-96-8	72
3			Phthalic acid, dec-2-yl isohexyl...	390	C24H38O4	1000356-94-1	72
4			Phthalic acid, di(oct-3-yl) ester	390	C24H38O4	1000377-72-3	64
5			Phthalic acid, monocyclohexyl ester	248	C14H16O4	007517-36-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062319.D
Acq On : 8 Aug 2024 4:30
Operator : MA/JU
Sample : P3437-05
Misc :
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Instrument :
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ClientSampleId :

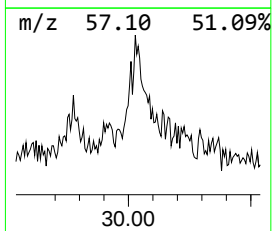
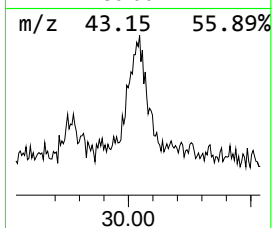
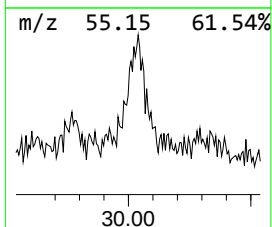
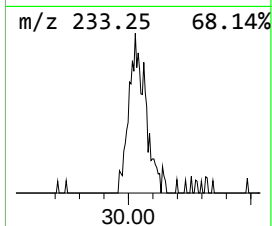
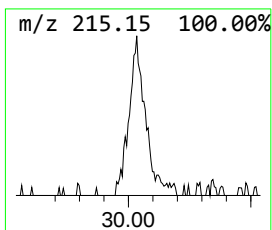
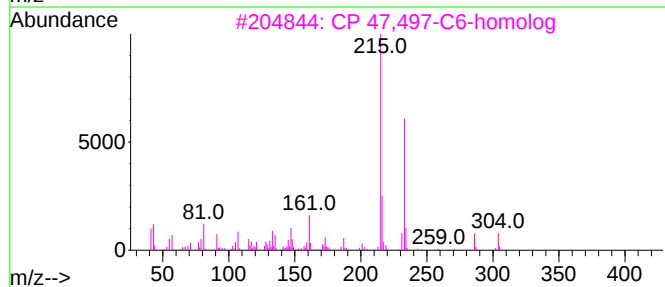
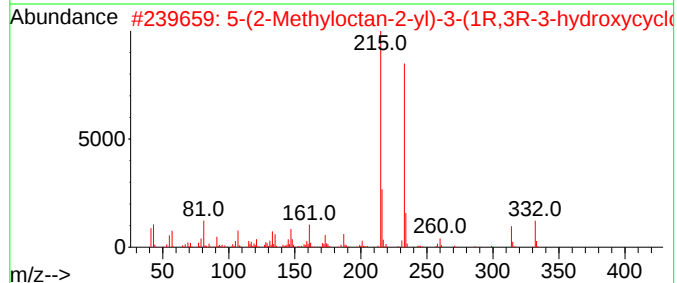
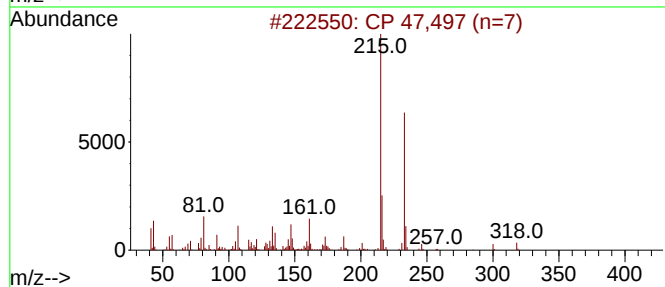
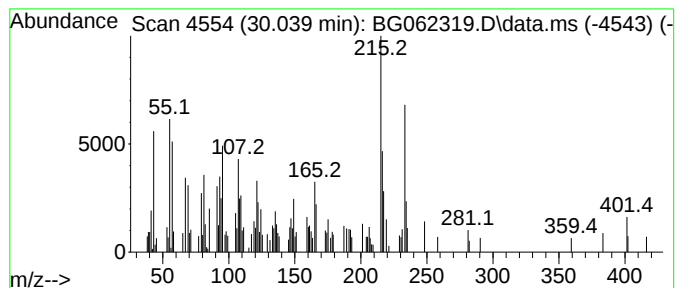
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.039	2.65 ng/ul	202639	Perylene-d12	24.641

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	CP	47,497	(n=7)	318	C21H34O2	070434-82-1	43
2	5-(2-Methyloctan-2-yl)-3-(1R,3R-...			332	C22H36O2	070434-92-3	38
3	CP	47,497	-C6-homolog	304	C20H32O2	070435-06-2	38
4	2-((1S,3R)-3-hydroxycyclohexyl)-...			332	C22H36O2	132296-11-8	38
5	2-Amino-5-bromo-3-fluorobenzoic	...		233	C7H5BrFNO2	874784-14-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062319.D
Acq On : 8 Aug 2024 4:30
Operator : MA/JU
Sample : P3437-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.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
n-Hexadecanoic ...	18.220	7.2	ng/ul	454574	4	17.316	1272240	20.0
1-Hexadecanol, ...	19.019	2.7	ng/ul	169439	4	17.316	1272240	20.0
Octadecanoic acid	19.489	3.1	ng/ul	217559	5	21.551	1411120	20.0
Dichloroacetic ...	21.234	2.3	ng/ul	165343	5	21.551	1411120	20.0
(4E,8E,13E)-1-(...	22.526	2.3	ng/ul	161780	5	21.551	1411120	20.0
1,4-Benzenedica...	22.720	3.0	ng/ul	212012	5	21.551	1411120	20.0
Phthalic acid, ...	23.231	8.7	ng/ul	667223	6	24.641	1532040	20.0
unknown-01	30.039	2.6	ng/ul	202639	6	24.641	1532040	20.0