

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
 Data File : BG057989.D
 Acq On : 4 Jul 2023 16:10
 Operator : CG/JU
 Sample : 03247-19
 Misc :
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DCGM5

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-BG070123.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG057989.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.118	3	5	23	rVB	2116927	2521197	65.72%	7.326%
2	3.376	46	49	53	rBV2	7727	9188	0.24%	0.027%
3	3.793	115	120	131	rBV	31858	58493	1.52%	0.170%
4	3.899	133	138	143	rVB2	13073	21168	0.55%	0.062%
5	4.028	155	160	165	rVB	17017	25784	0.67%	0.075%
6	4.346	210	214	218	rVB	9041	11347	0.30%	0.033%
7	5.168	350	354	360	rVB	15595	23773	0.62%	0.069%
8	6.619	596	601	608	rVB2	13030	21704	0.57%	0.063%
9	6.931	651	654	661	rBV4	4905	9431	0.25%	0.027%
10	7.107	675	684	696	rBV	138011	246347	6.42%	0.716%
11	7.219	696	703	706	rBV	14252	23923	0.62%	0.070%
12	7.266	706	711	718	rVB	121034	192995	5.03%	0.561%
13	7.471	739	746	753	rBV	143517	248245	6.47%	0.721%
14	7.941	819	826	833	rBV	220541	358512	9.35%	1.042%
15	8.646	940	946	954	rBV	130916	226573	5.91%	0.658%
16	9.099	1016	1023	1032	rBV	149256	262146	6.83%	0.762%
17	9.821	1139	1146	1155	rVB	117107	210343	5.48%	0.611%
18	10.051	1180	1185	1191	rVB4	8550	16736	0.44%	0.049%
19	10.362	1230	1238	1249	rBV	180770	325102	8.47%	0.945%
20	10.744	1295	1303	1316	rVB	336349	606614	15.81%	1.763%
21	10.879	1316	1326	1334	rBV	33245	69009	1.80%	0.201%
22	12.195	1544	1550	1561	rVB	75316	129497	3.38%	0.376%
23	13.458	1759	1765	1775	rBV5	19579	38541	1.00%	0.112%
24	13.893	1834	1839	1844	rVB3	20956	28396	0.74%	0.083%
25	13.975	1846	1853	1859	rVV	339545	480447	12.52%	1.396%
26	14.269	1896	1903	1911	rVV	384541	609463	15.89%	1.771%
27	14.334	1911	1914	1921	rVB4	5899	8949	0.23%	0.026%
28	14.416	1921	1928	1932	rBV5	6861	11334	0.30%	0.033%
29	14.457	1932	1935	1941	rVB2	6475	9277	0.24%	0.027%
30	14.575	1948	1955	1962	rBV	522699	812649	21.18%	2.361%
31	14.633	1962	1965	1979	rVB2	17133	30668	0.80%	0.089%
32	14.774	1982	1989	1994	rBV2	78769	138631	3.61%	0.403%
33	15.233	2060	2067	2071	rBV4	7544	11136	0.29%	0.032%
34	15.480	2101	2109	2113	rVV4	11805	20595	0.54%	0.060%
35	15.562	2117	2123	2134	rVV	518814	809055	21.09%	2.351%
36	15.679	2138	2143	2150	rVV	103351	153842	4.01%	0.447%

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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-BG070123.MA.M
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37	15.809	2161	2165	2170	rVB6	7088	12808	0.33%	0.037%
38	15.926	2179	2185	2190	rBV	62272	87131	2.27%	0.253%
39	16.026	2195	2202	2209	rVB8	10116	27138	0.71%	0.079%
40	16.132	2215	2220	2225	rVB6	10926	16962	0.44%	0.049%
41	16.190	2225	2230	2236	rBV7	7137	12924	0.34%	0.038%
42	16.279	2240	2245	2251	rVB7	10039	21033	0.55%	0.061%
43	16.414	2263	2268	2270	rBV5	13646	20354	0.53%	0.059%
44	16.449	2270	2274	2280	rVV2	19774	35709	0.93%	0.104%
45	17.019	2366	2371	2375	rBV2	94906	130339	3.40%	0.379%
46	17.060	2375	2378	2382	rVB4	9065	10020	0.26%	0.029%
47	17.201	2396	2402	2405	rBV5	10926	21937	0.57%	0.064%
48	17.266	2410	2413	2415	rBV4	8814	11226	0.29%	0.033%
49	17.319	2415	2422	2428	rVV	617010	962056	25.08%	2.796%
50	17.413	2432	2438	2445	rVB	414414	653281	17.03%	1.898%
51	17.483	2445	2450	2453	rBV6	5571	10546	0.27%	0.031%
52	17.577	2461	2466	2472	rBV5	12615	27807	0.72%	0.081%
53	17.800	2500	2504	2511	rBV3	7737	12731	0.33%	0.037%
54	17.977	2523	2534	2538	rBV9	16472	33489	0.87%	0.097%
55	18.071	2543	2550	2558	rBV5	40958	85967	2.24%	0.250%
56	18.141	2558	2562	2567	rBV	32654	47111	1.23%	0.137%
57	18.200	2567	2572	2582	rBV	393165	571951	14.91%	1.662%
58	18.394	2601	2605	2610	rVB2	17141	22991	0.60%	0.067%
59	18.458	2612	2616	2618	rVV4	9083	11599	0.30%	0.034%
60	18.494	2618	2622	2625	rVV2	13146	16667	0.43%	0.048%
61	18.541	2626	2630	2635	rVB3	22474	36417	0.95%	0.106%
62	18.623	2640	2644	2648	rVB6	16482	20696	0.54%	0.060%
63	18.693	2652	2656	2659	rBV6	9773	16371	0.43%	0.048%
64	18.782	2669	2671	2675	rVB5	11279	12505	0.33%	0.036%
65	18.946	2695	2699	2702	rBV2	16473	19884	0.52%	0.058%
66	19.122	2726	2729	2734	rVB3	30813	38381	1.00%	0.112%
67	19.216	2740	2745	2751	rBV3	31960	60283	1.57%	0.175%
68	19.263	2751	2753	2757	rVB5	8151	8632	0.23%	0.025%
69	19.328	2761	2764	2767	rBV3	65069	95169	2.48%	0.277%
70	19.369	2767	2771	2776	rVB	70554	134045	3.49%	0.390%
71	19.475	2782	2789	2798	rBV2	96918	163735	4.27%	0.476%
72	19.616	2811	2813	2819	rVB4	13169	13236	0.35%	0.038%
73	19.704	2822	2828	2838	rVB	632689	957645	24.96%	2.783%
74	19.857	2849	2854	2860	rBV	219918	286652	7.47%	0.833%
75	20.209	2909	2914	2915	rBV2	66525	86189	2.25%	0.250%
76	20.227	2915	2917	2924	rVB2	96141	129904	3.39%	0.377%

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77	20.562	2968	2974	2979	rBV4	45713	83242	2.17%	0.242%
78	20.668	2988	2992	2995	rBV2	16106	21857	0.57%	0.064%
79	20.720	2997	3001	3005	rVB2	56854	78532	2.05%	0.228%
80	20.897	3029	3031	3039	rVB5	29485	48424	1.26%	0.141%
81	21.044	3052	3056	3062	rBV2	31488	49352	1.29%	0.143%
82	21.214	3080	3085	3096	rBV	373536	574315	14.97%	1.669%
83	21.572	3139	3146	3151	rBV	580975	1012079	26.38%	2.941%
84	21.755	3174	3177	3183	rVB2	51797	77205	2.01%	0.224%
85	21.984	3210	3216	3227	rVB2	218206	399041	10.40%	1.160%
86	22.377	3273	3283	3295	rBV3	360249	1038011	27.06%	3.016%
87	23.024	3386	3393	3399	rVB3	90321	219206	5.71%	0.637%
88	23.376	3447	3453	3462	rVB2	162159	317258	8.27%	0.922%
89	23.823	3521	3529	3536	rBV	920246	1934701	50.43%	5.622%
90	23.887	3536	3540	3553	rVB2	128900	310235	8.09%	0.901%
91	24.516	3639	3647	3657	rBV3	281654	749003	19.52%	2.176%
92	24.739	3676	3685	3698	rVB2	447233	1286918	33.55%	3.740%
93	25.262	3765	3774	3784	rBV	252563	665587	17.35%	1.934%
94	25.861	3866	3876	3888	rVB	683775	2027872	52.86%	5.893%
95	25.991	3890	3898	3909	rBV4	139113	505307	13.17%	1.468%
96	27.195	4096	4103	4115	rVB2	91942	311203	8.11%	0.904%
97	27.977	4223	4236	4253	rVB2	503191	1979690	51.60%	5.753%
98	28.805	4365	4377	4404	rVB3	276254	1452292	37.86%	4.220%
99	29.968	4565	4575	4608	rVB4	313248	1711891	44.62%	4.974%
100	31.461	4814	4829	4851	rVB7	661084	3836302	100.00%	11.147%

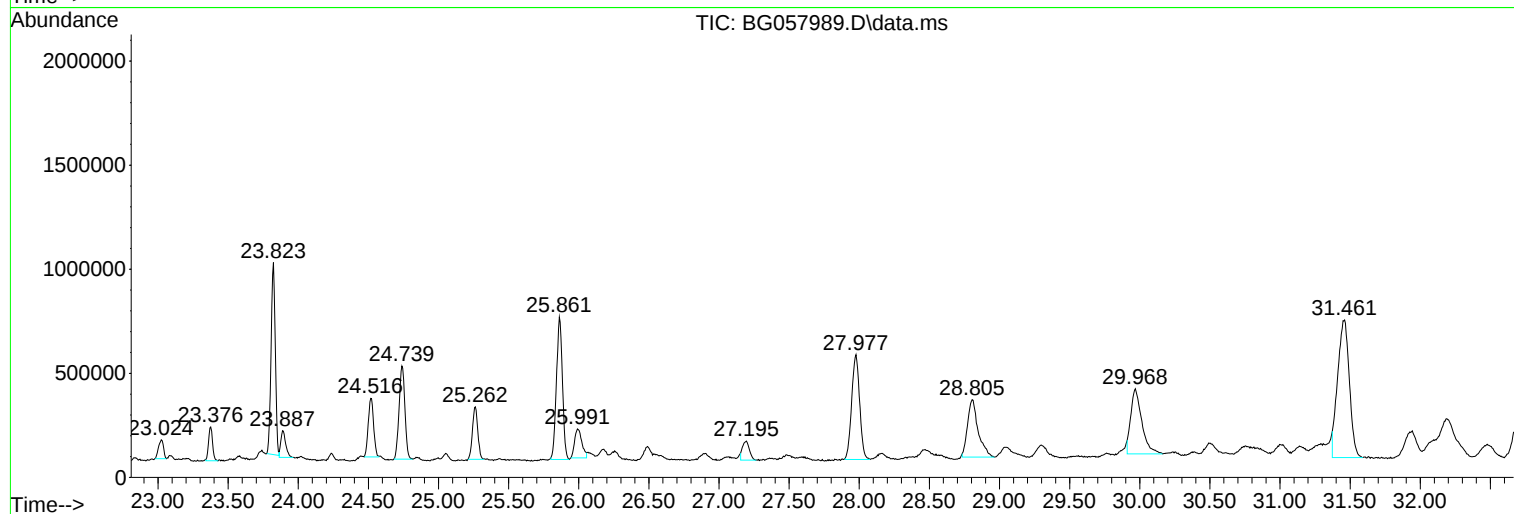
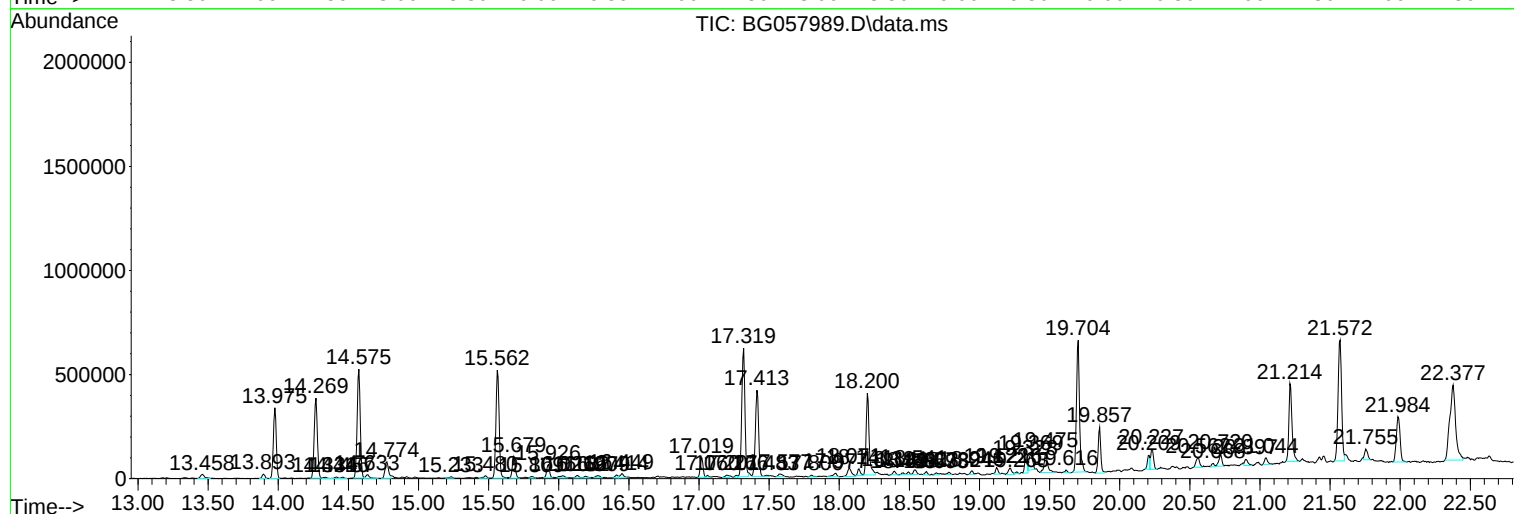
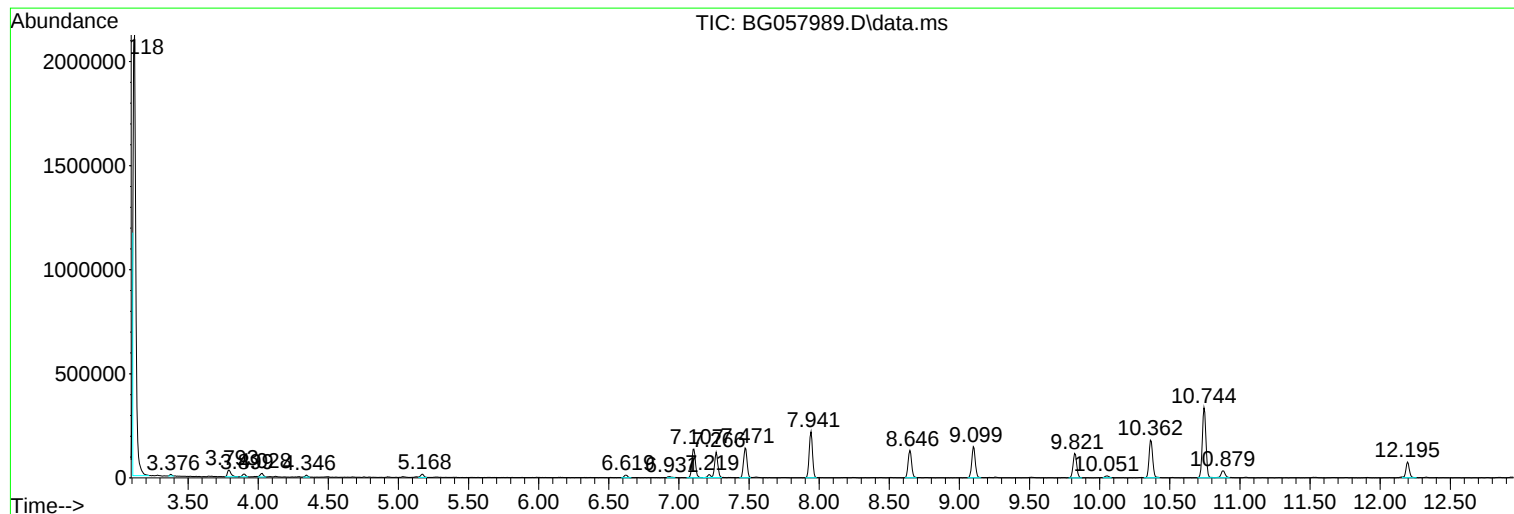
Sum of corrected areas: 34414154

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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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



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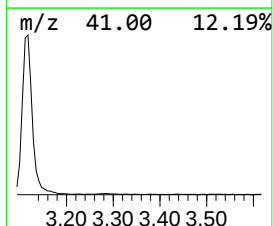
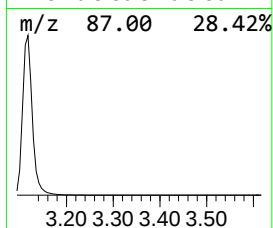
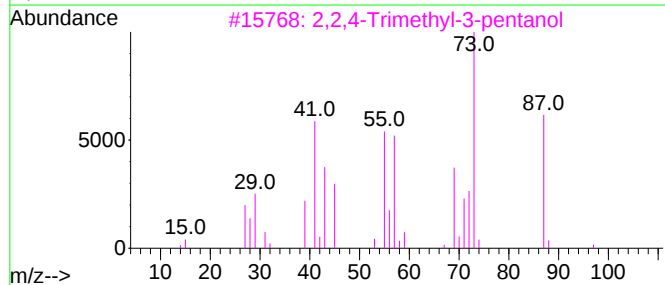
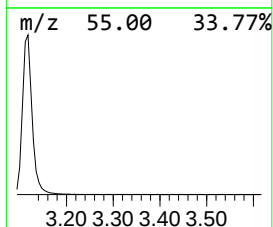
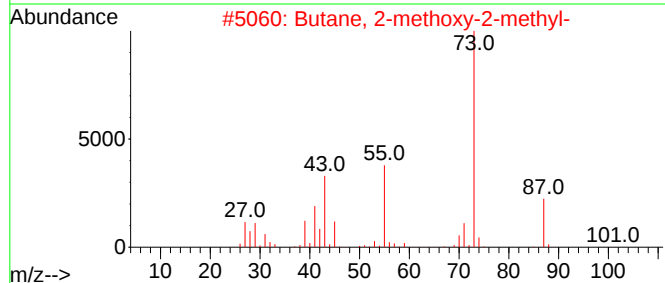
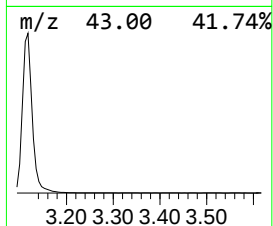
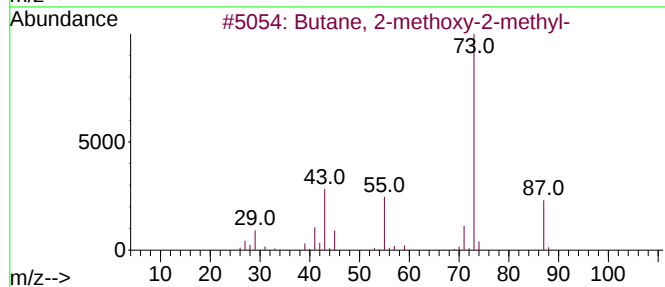
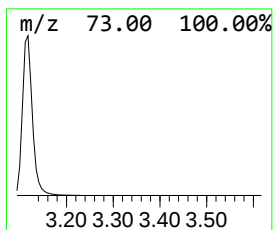
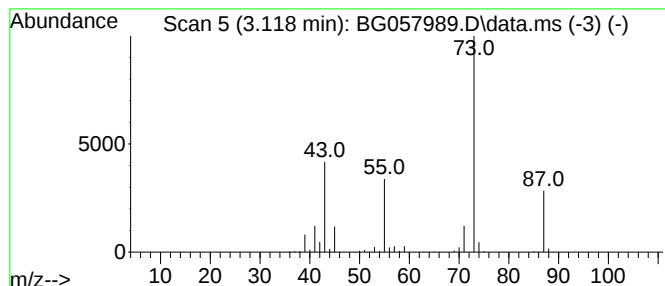
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.118	140.65 ng/ul	2521200	1,4-Dichlorobenzene-d4	7.941

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35



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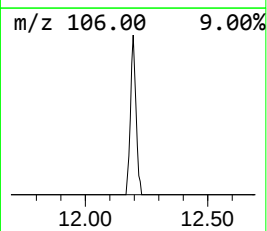
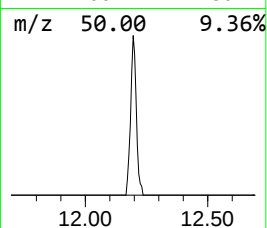
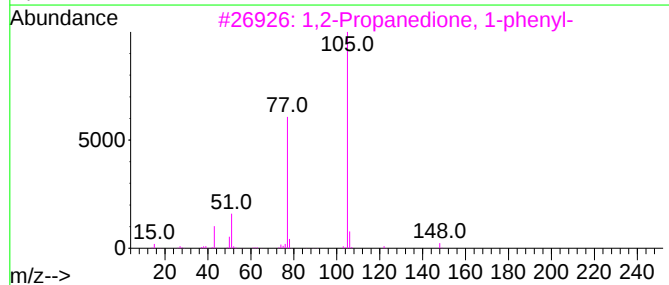
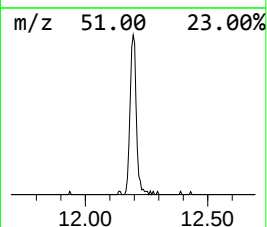
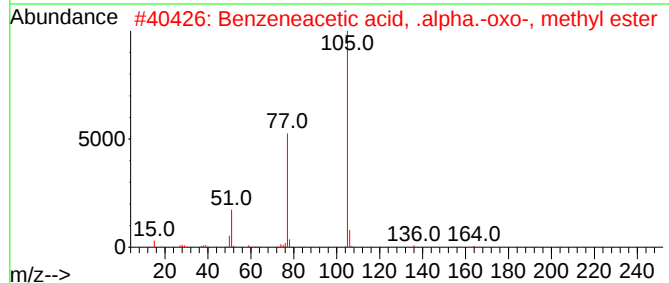
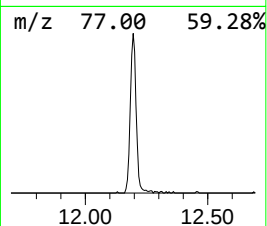
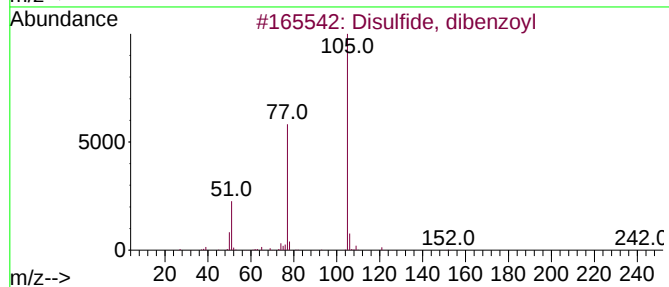
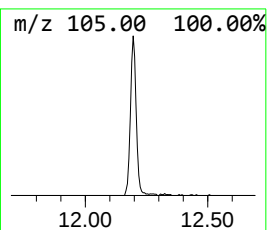
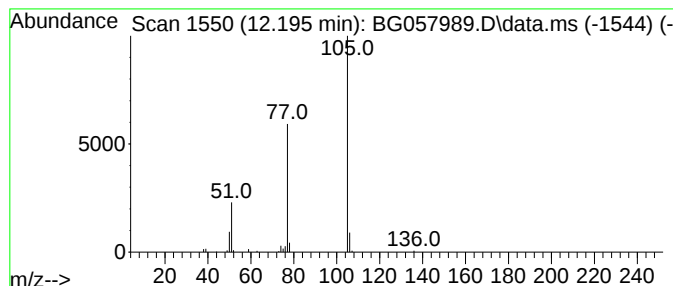
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Disulfide, dibenzoyl Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.195	4.27 ng/ul	129497	Naphthalene-d8	10.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	90
2			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	83
3			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	83
4			Phenylglyoxal	134	C8H6O2	001074-12-0	83
5			Benzoylformic acid	150	C8H6O3	000611-73-4	83



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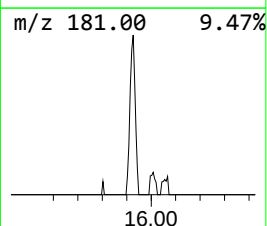
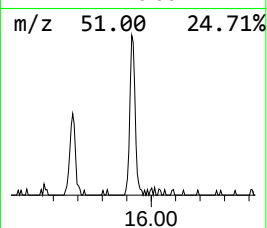
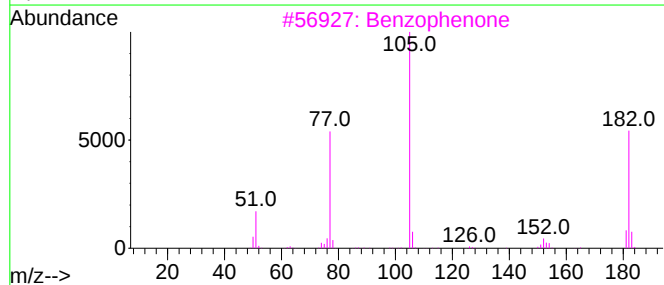
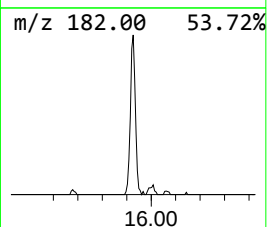
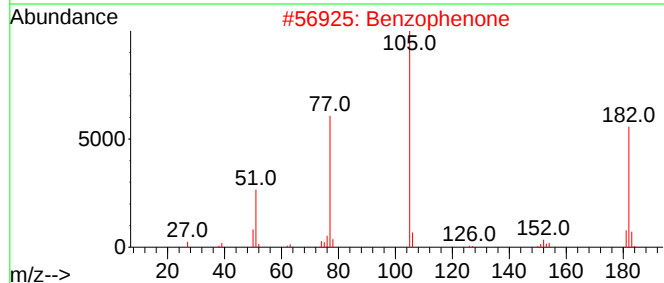
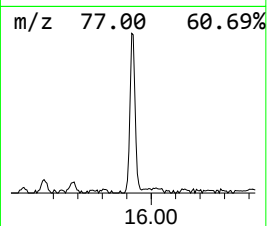
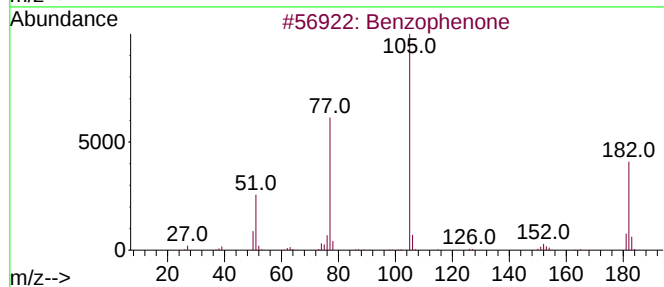
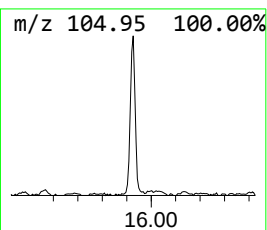
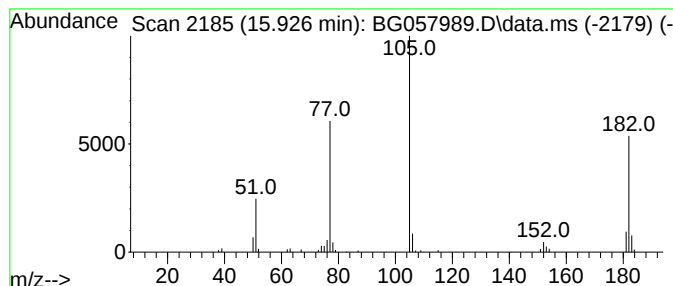
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 23

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.926	2.14 ng/ul	87131	Acenaphthene-d10	14.575

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzophenone	182	C13H10O	000119-61-9	96
3			Benzophenone	182	C13H10O	000119-61-9	95
4			Benzophenone	182	C13H10O	000119-61-9	91
5			Benzophenone	182	C13H10O	000119-61-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
Operator : CG/JU
Sample : 03247-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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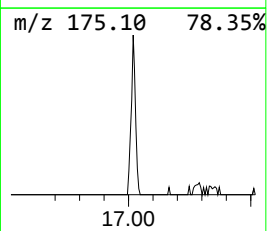
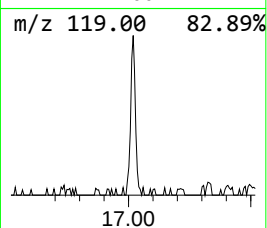
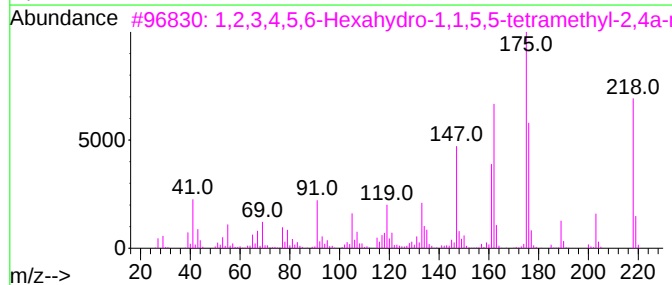
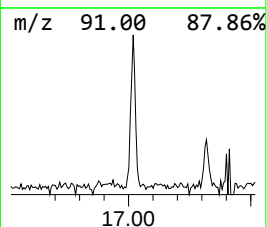
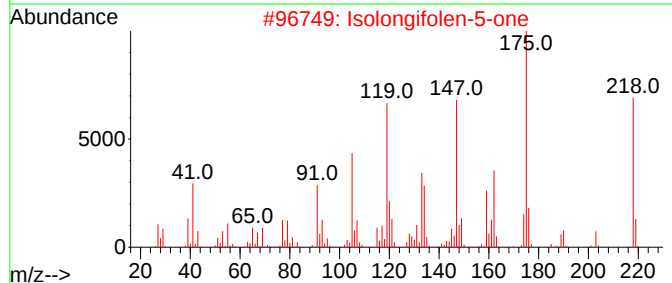
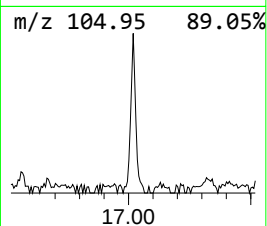
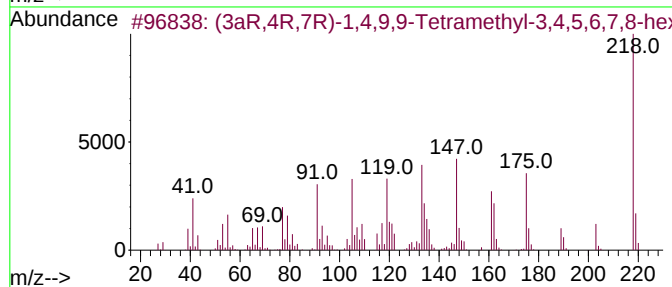
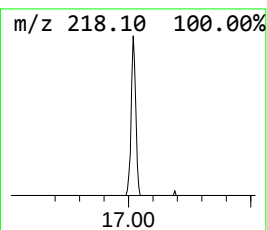
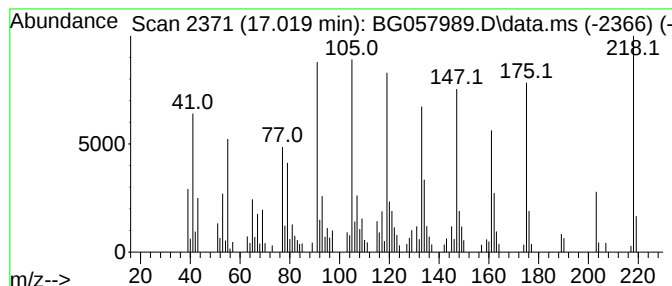
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (3aR,4R,7R)-1,4,9,9-Tetrame... Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.019	2.71 ng/ul	130339	Phenanthrene-d10	17.319

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(3aR,4R,7R)-1,4,9,9-Tetramethyl-...	218	C15H22O	003466-15-7	93
2			Isolongifolen-5-one	218	C15H22O	1000159-37-1	91
3			1,2,3,4,5,6-Hexahydro-1,1,5,5-te...	218	C15H22O	023747-14-0	87
4			2(3H)-Naphthalenone, 4,4a,5,6,7,...	218	C15H22O	019598-45-9	78
5			2,4a-Methanonaphthalen-7(4aH)-on...	218	C15H22O	026839-52-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
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Sample : 03247-19
Misc :
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Instrument :
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ClientSampleId :
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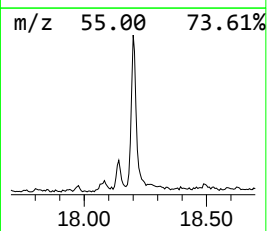
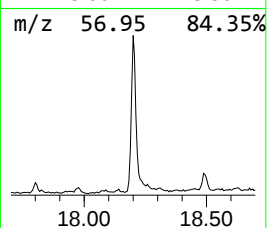
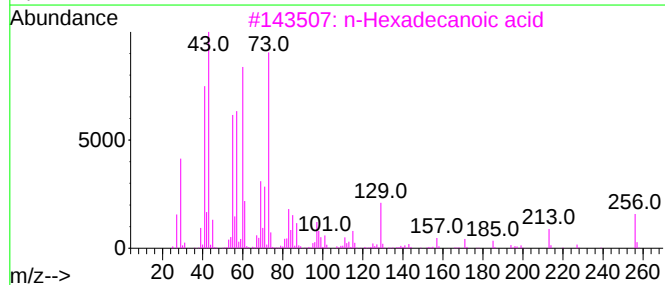
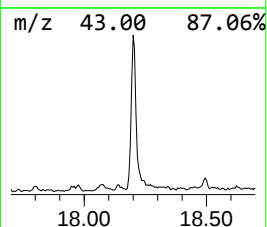
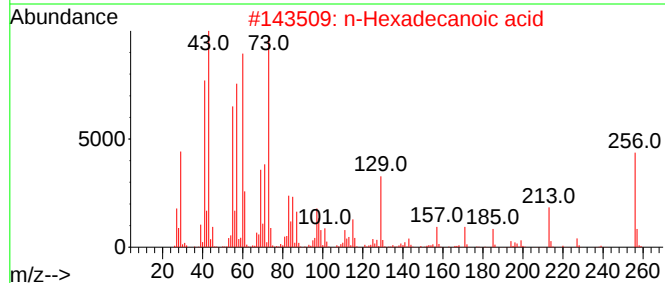
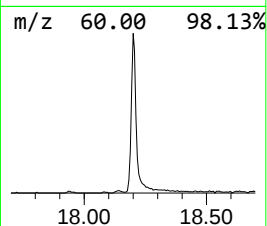
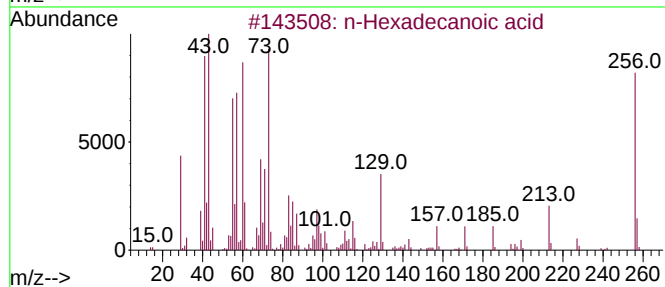
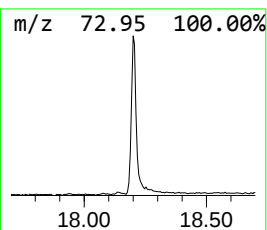
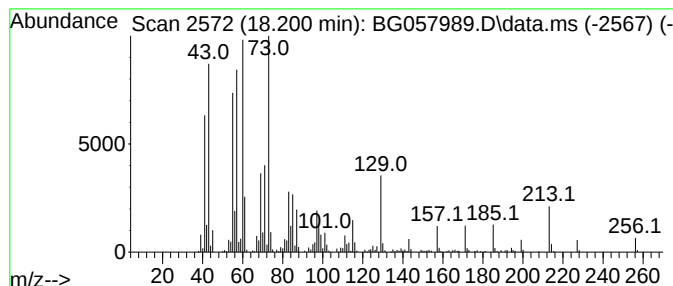
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.200	11.89 ng/ul	571951	Phenanthrene-d10	17.319

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
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Sample : 03247-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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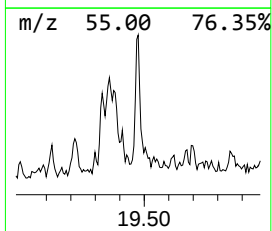
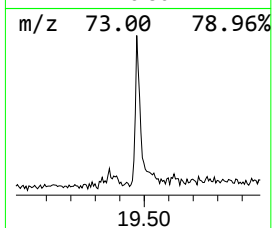
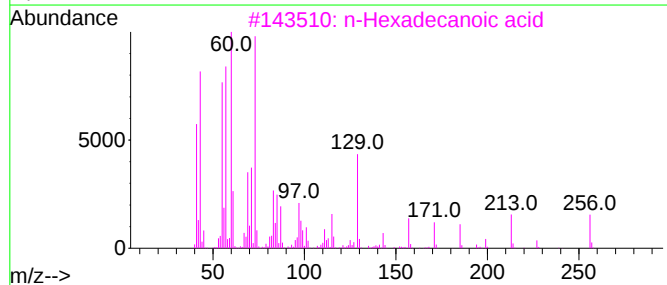
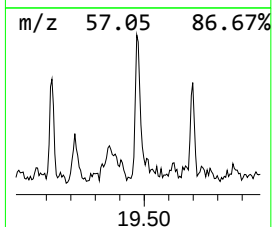
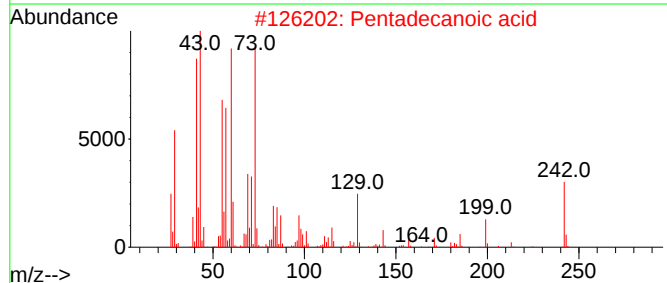
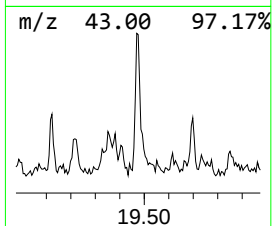
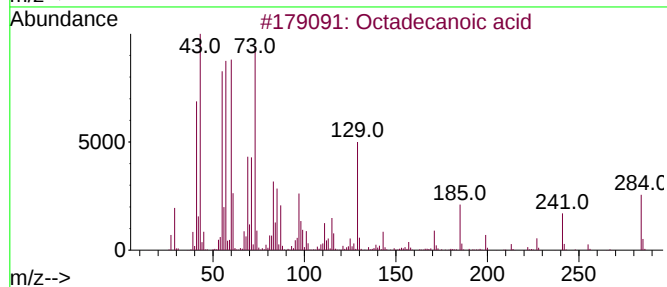
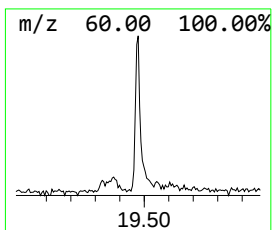
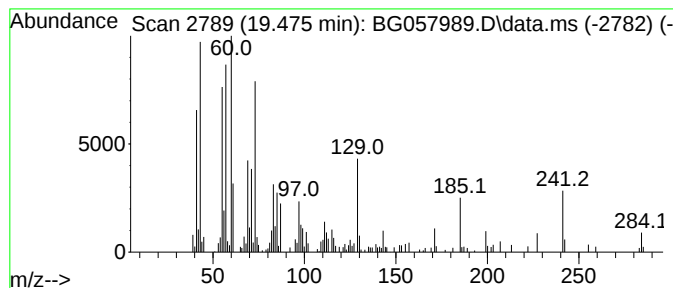
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.475	3.24 ng/ul	163735	Chrysene-d12	21.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Octadecanoic acid	284	C18H36O2	000057-11-4	86
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
Operator : CG/JU
Sample : 03247-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

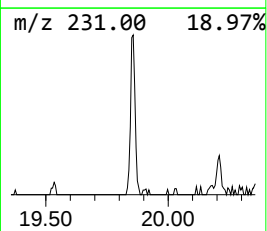
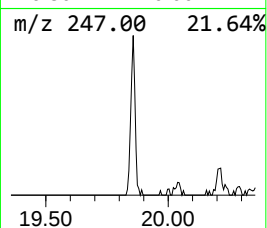
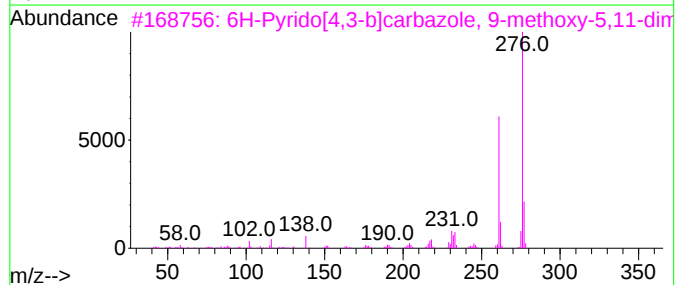
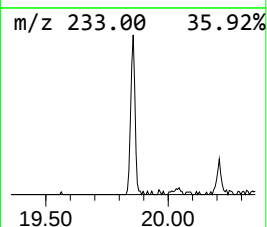
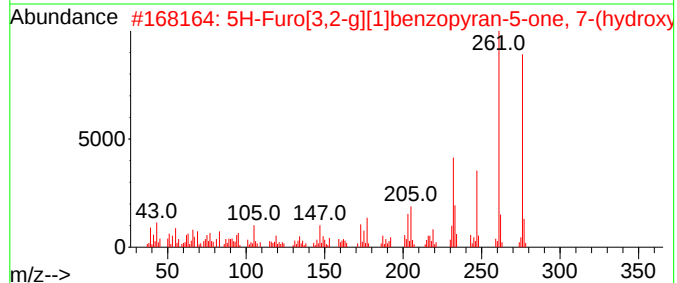
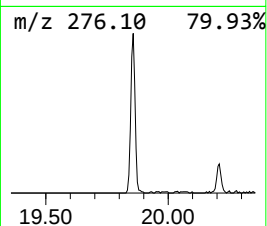
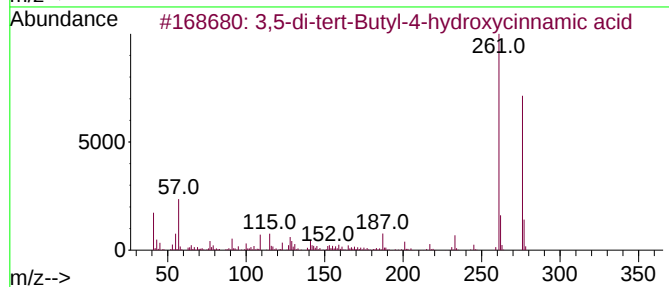
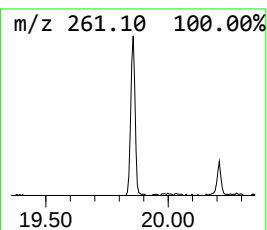
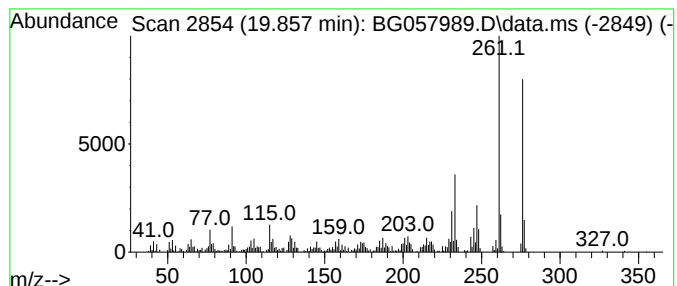
Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.857	5.66 ng/ul	286652	Chrysene-d12	21.572	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxycinna...	276	C17H24O3	022014-01-3	89
2	5H-Furo[3,2-g][1]benzopyran-5-on...	276	C14H12O6	000668-10-0	83
3	6H-Pyrido[4,3-b]carbazole, 9-met...	276	C18H16N2O	010371-86-5	72
4	5,6,7,8-Tetrahydrothieno[2,3-b]q...	276	C14H20N2SSi	1000496-40-4	64
5	5-[4-(Diethylamino)phenyl]-4-eth...	276	C14H20N4S	1000476-62-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
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Acq On : 4 Jul 2023 16:10
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Sample : 03247-19
Misc :
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Instrument :
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ClientSampleId :
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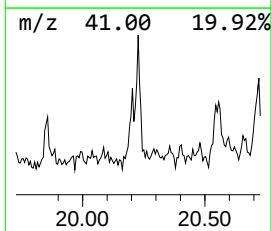
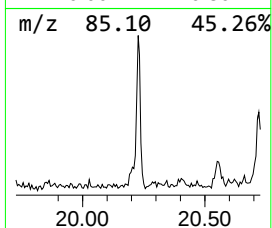
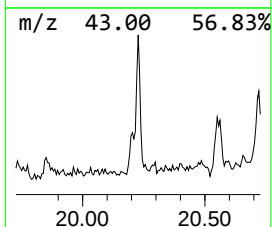
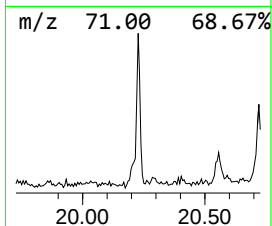
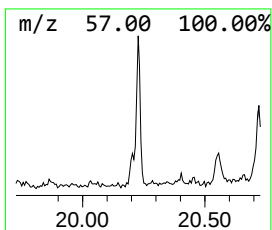
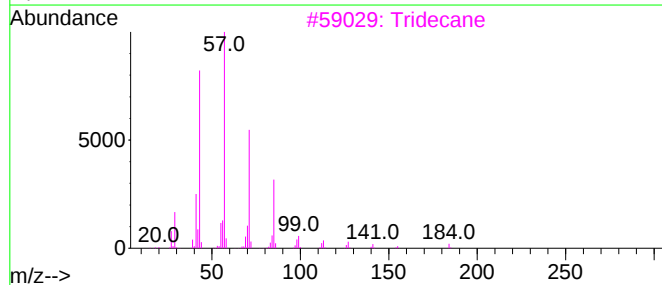
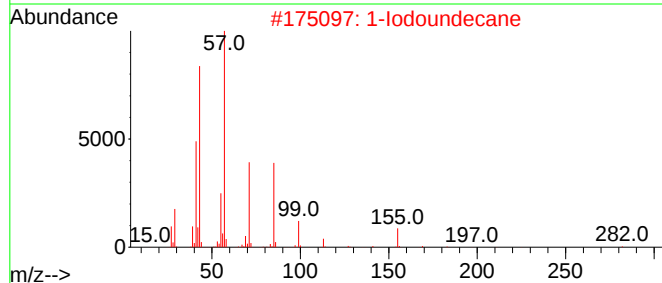
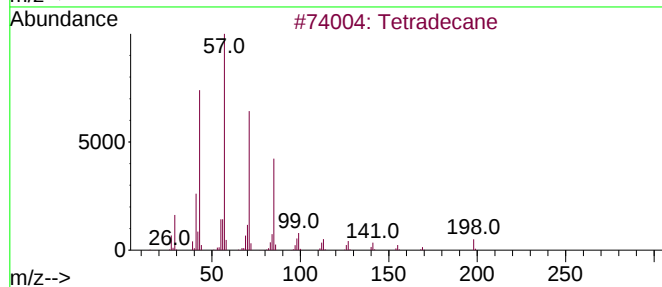
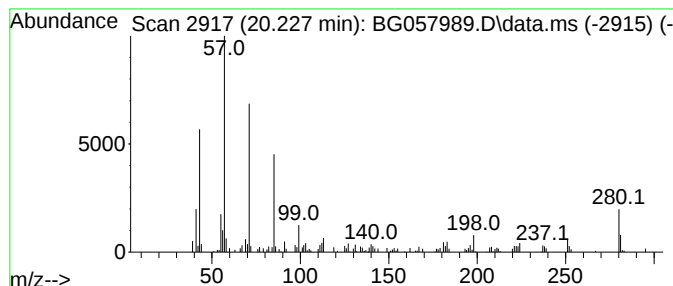
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Cyclic20.227 Concentration Rank 22

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.227	2.57 ng/ul	129904	Chrysene-d12	21.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	64
2			1-Iodoundecane	282	C11H23I	004282-44-4	62
3			Tridecane	184	C13H28	000629-50-5	62
4			Pentadecane	212	C15H32	000629-62-9	58
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
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Sample : 03247-19
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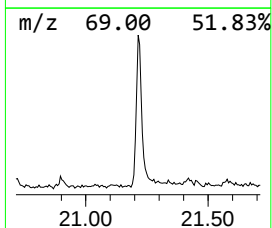
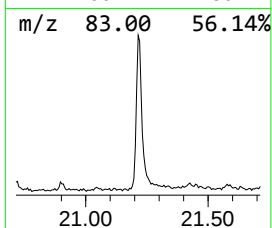
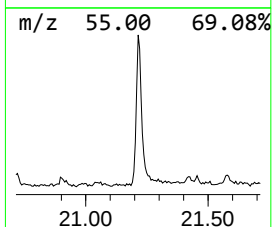
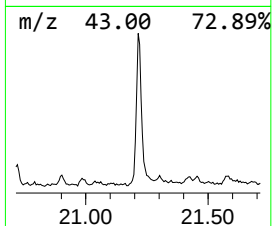
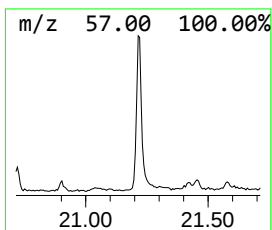
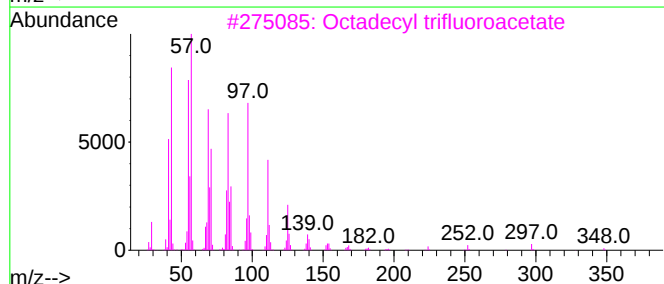
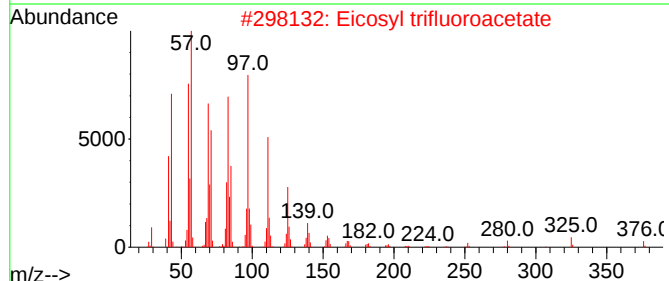
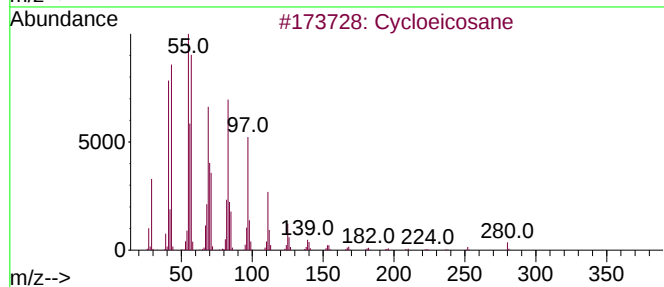
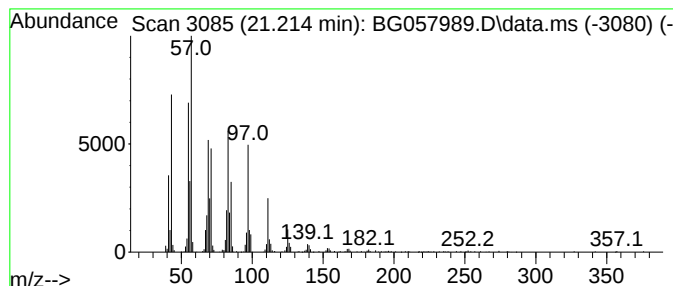
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 (DEL) Alkane: Cyclic21.214 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.214	11.35 ng/ul	574315	Chrysene-d12	21.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	96
2			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
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Misc :
ALS Vial : 47 Sample Multiplier: 1

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ClientSampleId :
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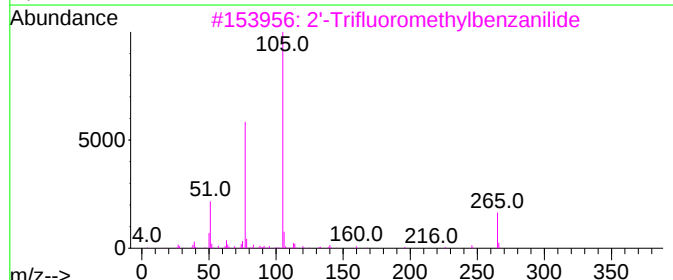
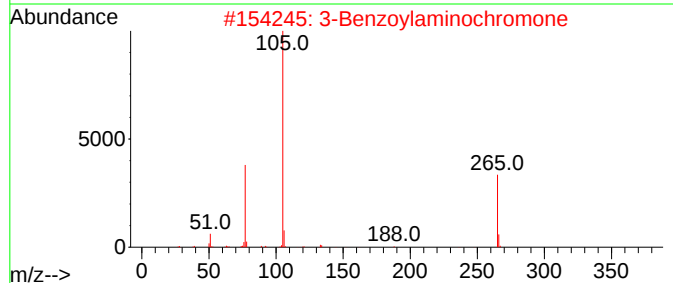
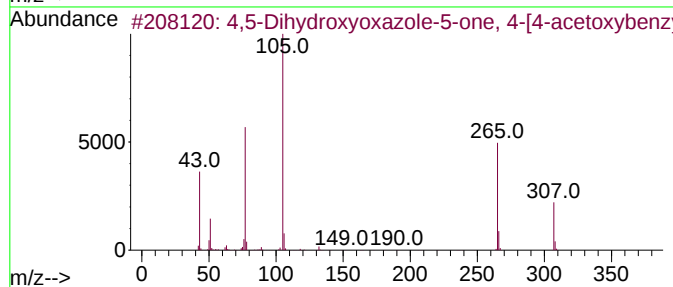
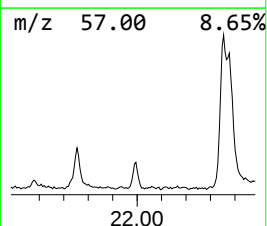
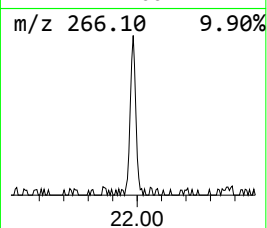
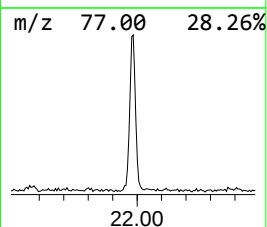
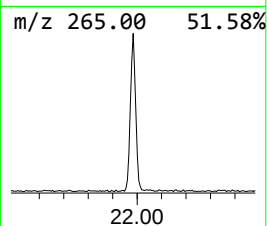
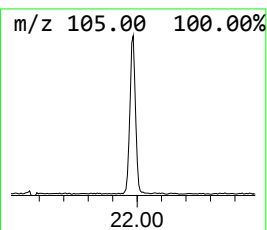
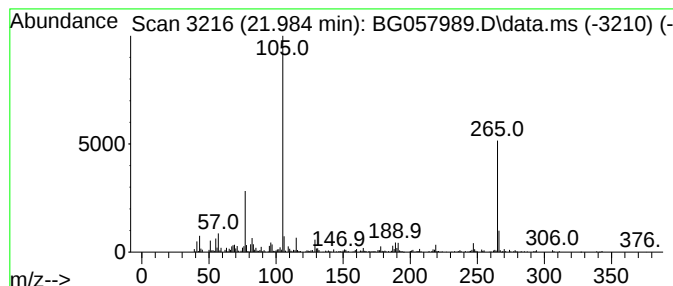
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 4,5-Dihydroxyoxazole-5-one,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.984	7.89 ng/ul	399041	Chrysene-d12	21.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,5-Dihydroxyoxazole-5-one, 4-[4...	307	C18H13NO4	1000130-54-7	64
2			3-Benzoylaminochromone	265	C16H11NO3	1000243-49-5	64
3			2'-Trifluoromethylbenzanilide	265	C14H10F3NO	001939-24-8	64
4			Benzene, 1-nitro-2-hydroxy-4-(p-...	265	C12H8ClNO4	027783-57-9	35
5			Cyclobutyl phenyl ketone	160	C11H12O	005407-98-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
Operator : CG/JU
Sample : 03247-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM5

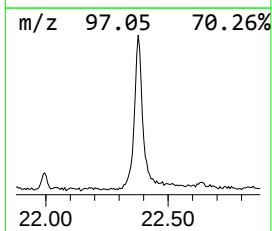
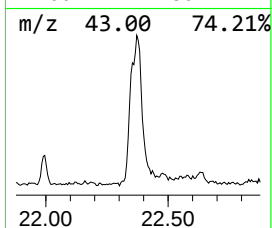
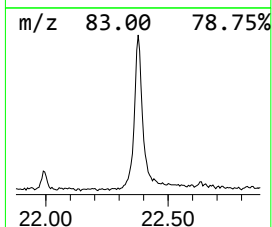
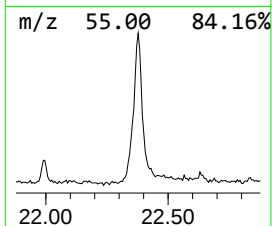
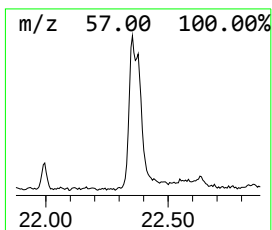
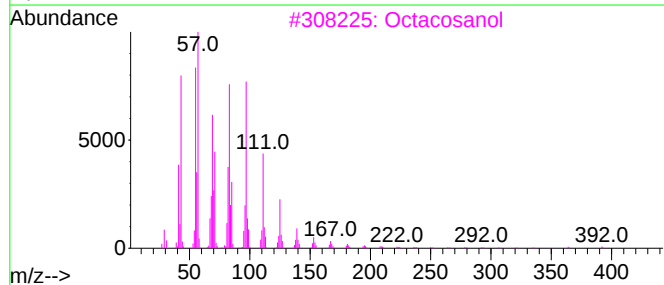
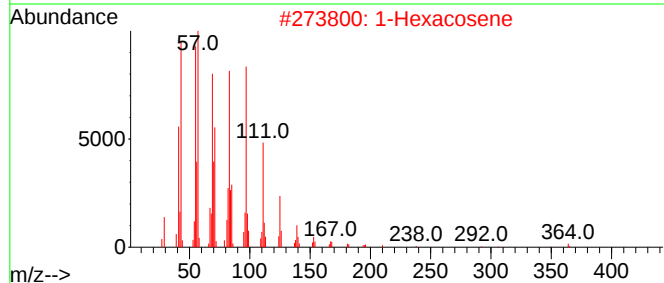
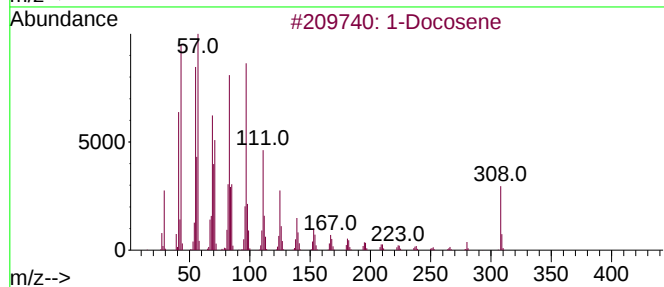
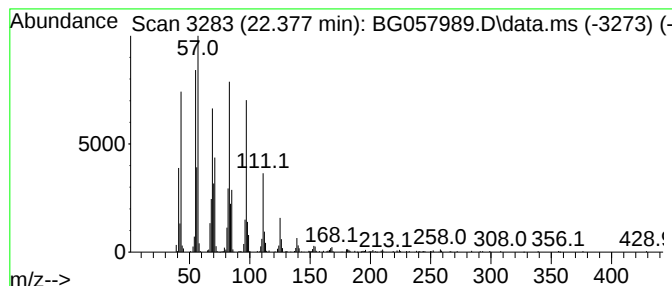
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.377	20.51 ng/ul	1038010	Chrysene-d12	21.572

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	95
2	1-Hexacosene		364	C26H52	018835-33-1	94
3	Octacosanol		410	C28H58O	000557-61-9	94
4	Nonacos-1-ene		406	C29H58	018835-35-3	94
5	1-Heneicosanol		312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
Operator : CG/JU
Sample : 03247-19
Misc :
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Instrument :
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ClientSampleId :
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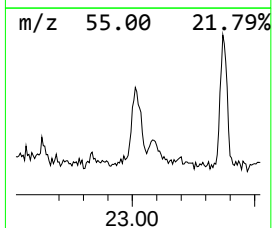
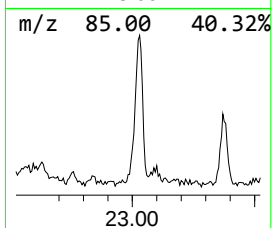
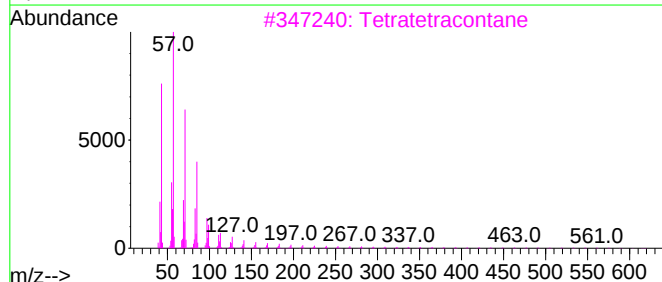
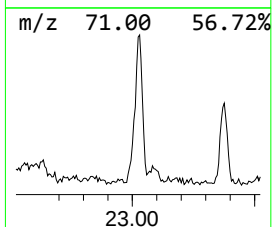
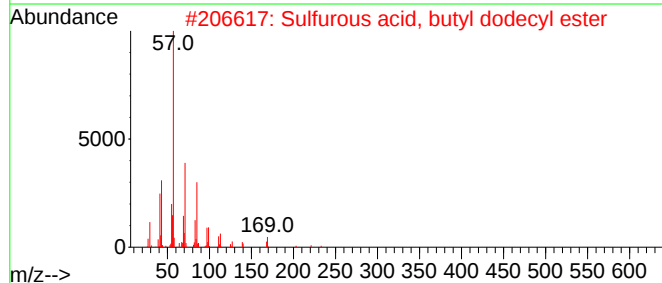
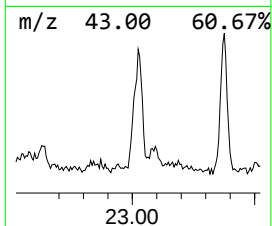
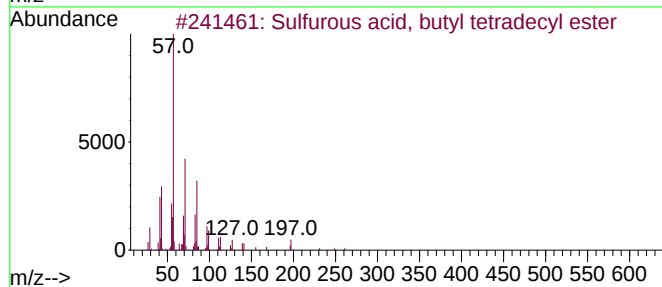
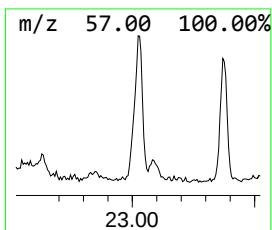
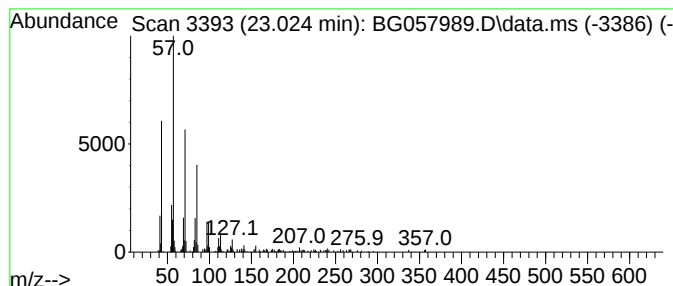
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Quant Title : SVOA CALIBRATION

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

Peak Number 12 Sulfurous acid, butyl tetra... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.024	4.33 ng/ul	219206	Chrysene-d12	21.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	90
2			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	87
3			Tetratetracontane	619	C44H90	007098-22-8	86
4			Heneicosane	296	C21H44	000629-94-7	83
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
Operator : CG/JU
Sample : 03247-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

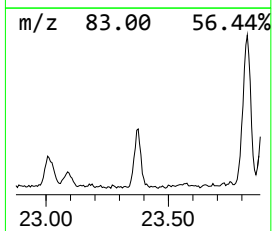
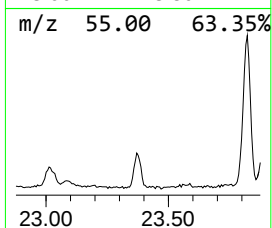
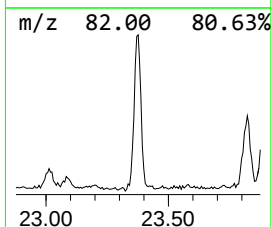
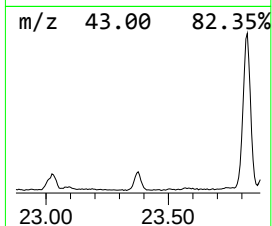
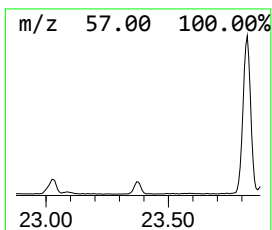
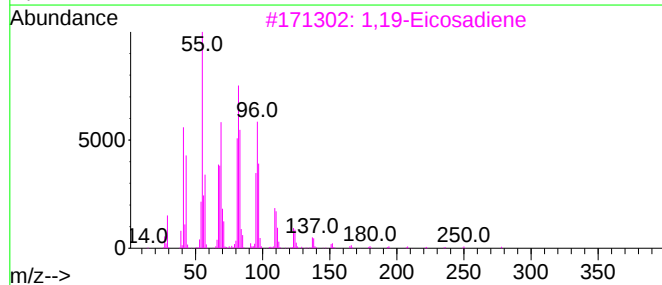
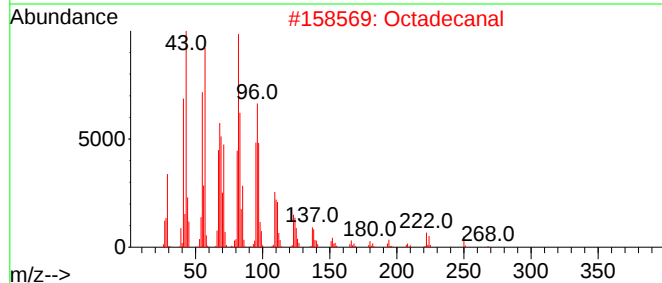
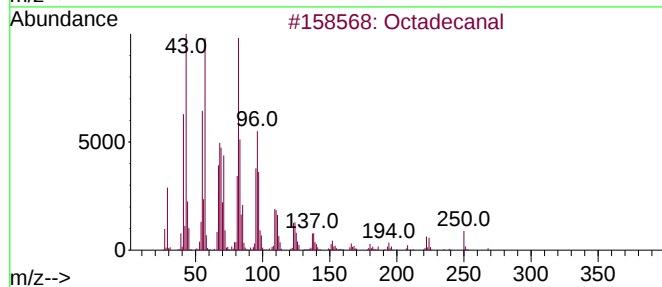
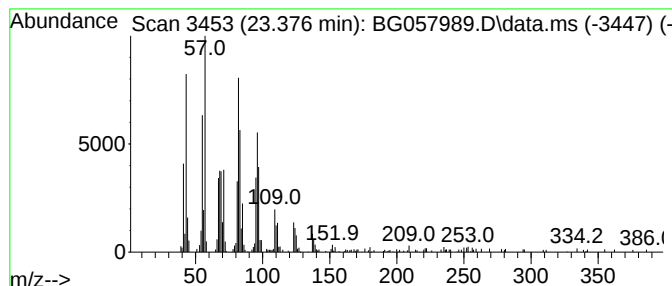
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 13 Octadecanal Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.376	4.93 ng/ul	317258	Perylene-d12	24.739	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	90
2	Octadecanal	268	C18H36O	000638-66-4	87
3	1,19-Eicosadiene	278	C20H38	014811-95-1	81
4	Pentadecanal-	226	C15H30O	002765-11-9	80
5	11-Tetradecyn-1-ol acetate	252	C16H28O2	033925-72-3	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
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Sample : 03247-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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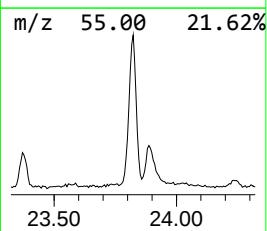
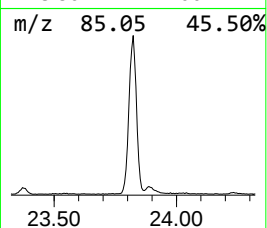
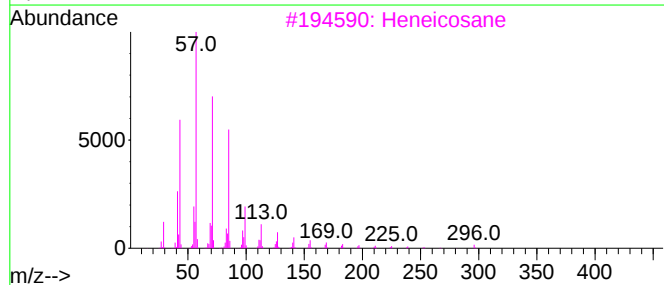
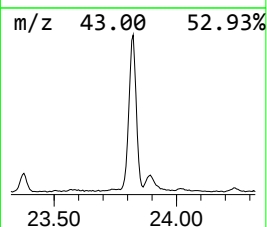
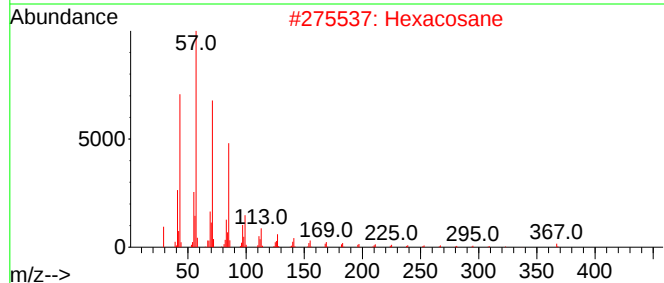
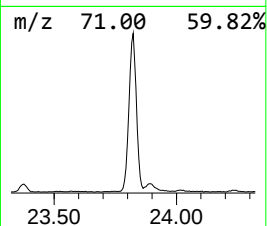
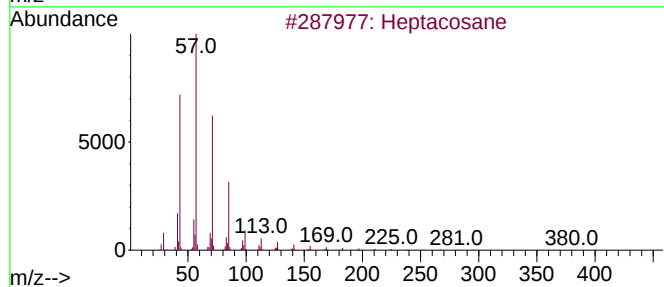
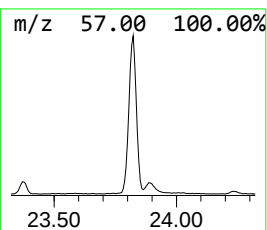
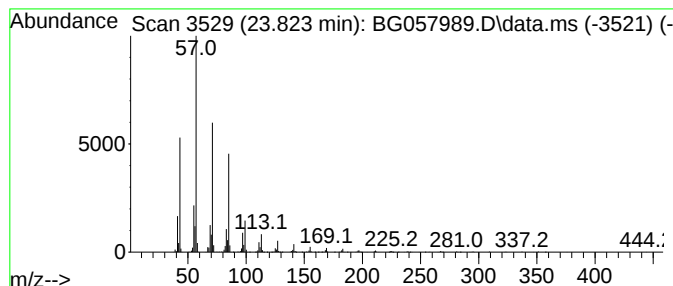
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Quant Title : SVOA CALIBRATION

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

Peak Number 14 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.823	30.07 ng/ul	1934700	Perylene-d12	24.739

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Pentacosane	352	C25H52	000629-99-2	90
5		Nonadecane	268	C19H40	000629-92-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
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Acq On : 4 Jul 2023 16:10
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Sample : 03247-19
Misc :
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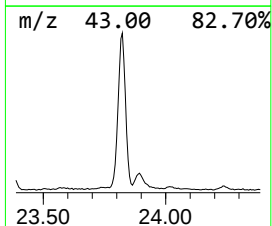
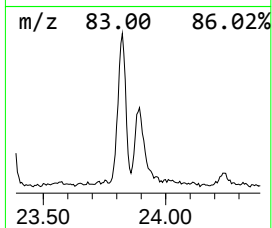
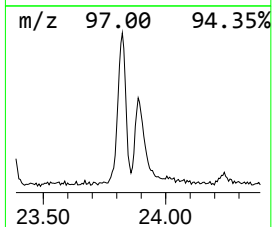
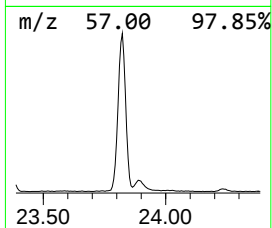
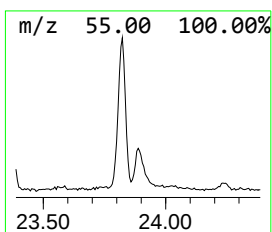
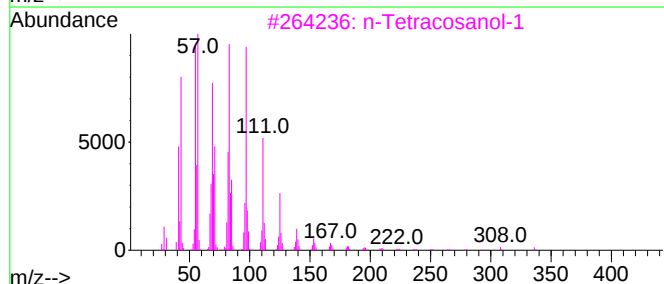
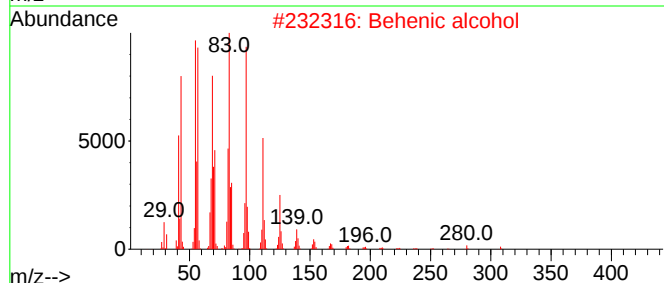
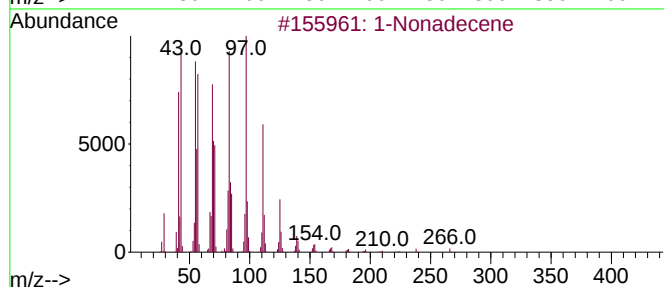
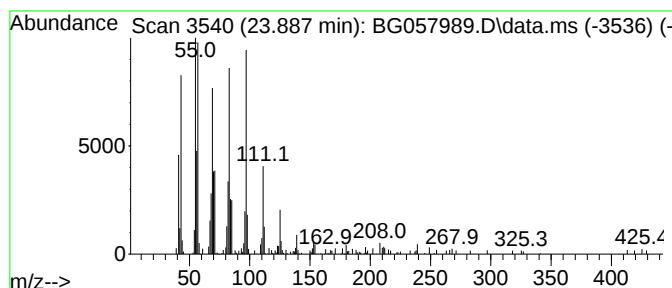
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 15 (DEL) Alkane: Straight-Chai... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.887	4.82 ng/ul	310235	Perylene-d12		24.739	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	98
2	Behenic alcohol		326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1		354	C24H50O	000506-51-4	95
4	1-Heneicosanol		312	C21H44O	015594-90-8	94
5	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
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Acq On : 4 Jul 2023 16:10
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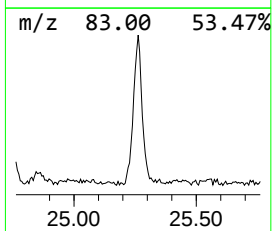
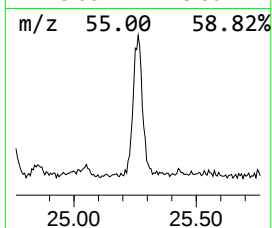
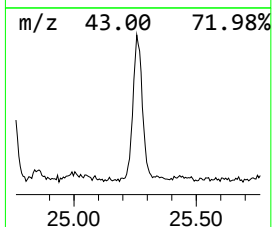
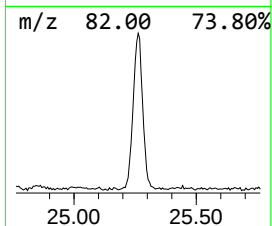
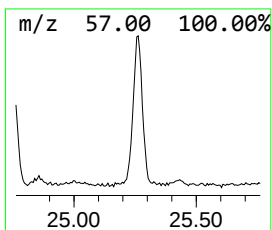
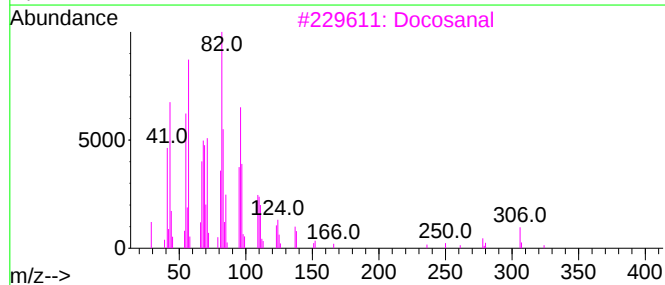
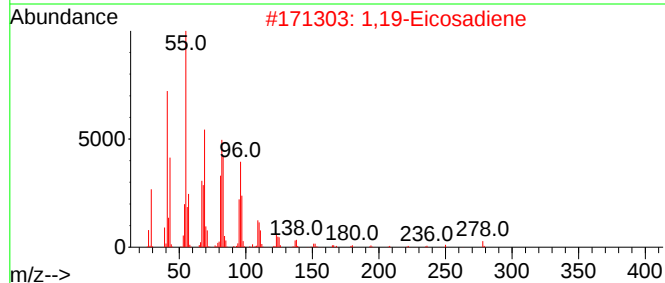
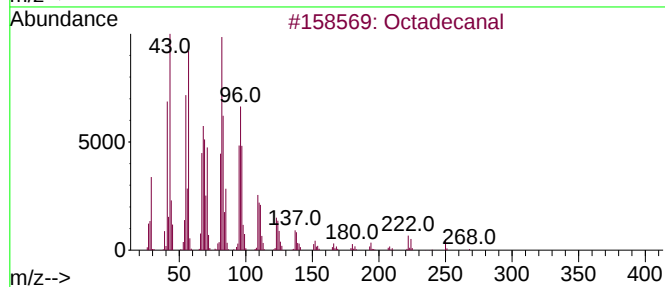
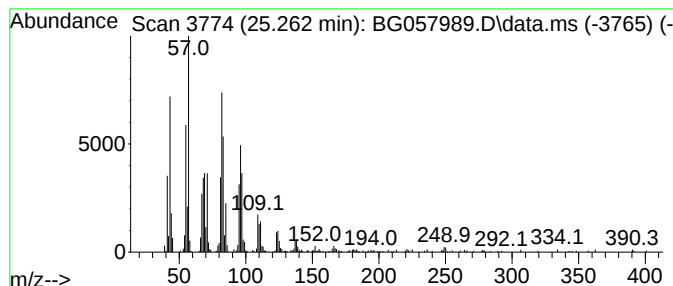
Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 16 1,19-Eicosadiene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.262	10.34 ng/ul	665587	Perylene-d12	24.739	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	1,19-Eicosadiene	278	C20H38	014811-95-1	87
3	Docosanal	324	C22H44O	057402-36-5	87
4	Octadecanal	268	C18H36O	000638-66-4	83
5	Eicosanal-	296	C20H40O	002400-66-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
Operator : CG/JU
Sample : 03247-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DCGM5

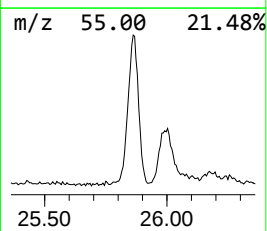
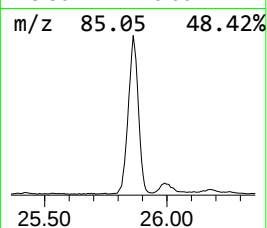
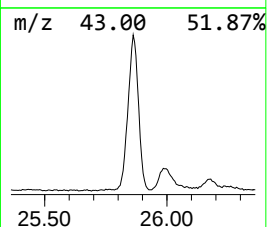
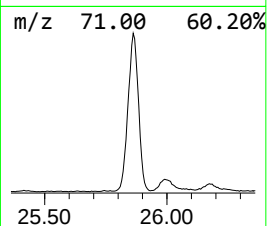
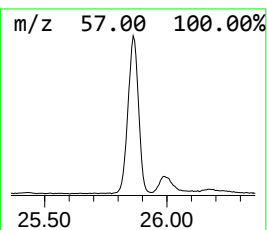
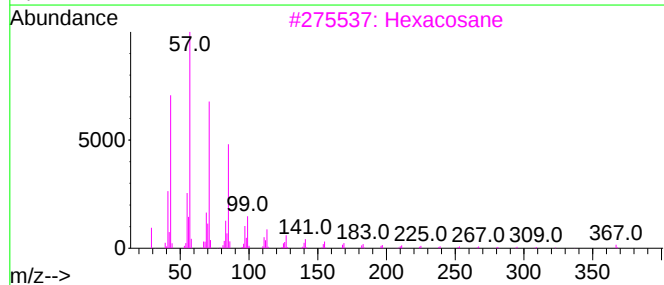
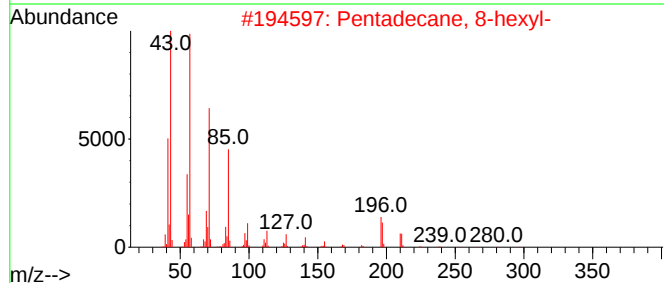
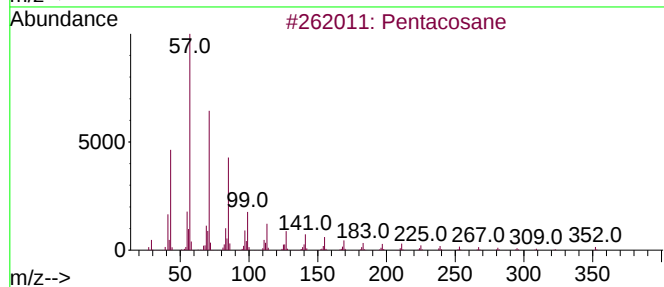
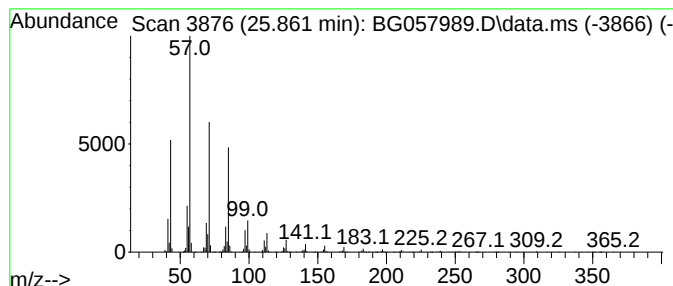
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Quant Title : SVOA CALIBRATION

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

Peak Number 17 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.861	31.52 ng/ul	2027870	Perylene-d12	24.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	96
2			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
3			Hexacosane	366	C26H54	000630-01-3	91
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5			Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
Operator : CG/JU
Sample : 03247-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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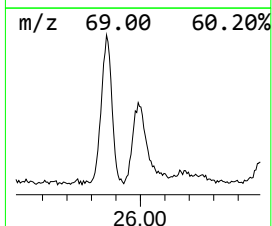
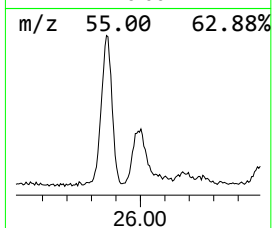
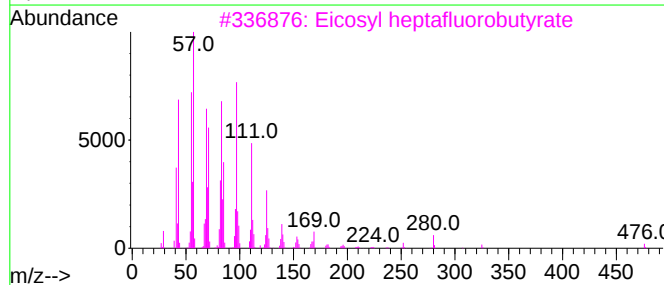
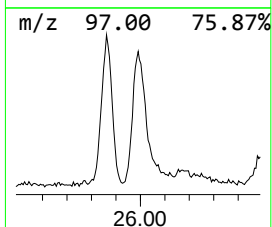
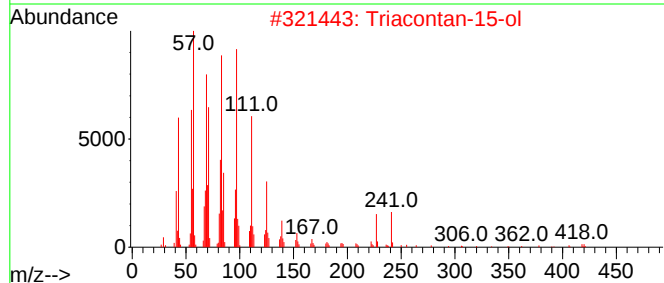
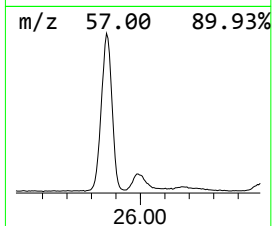
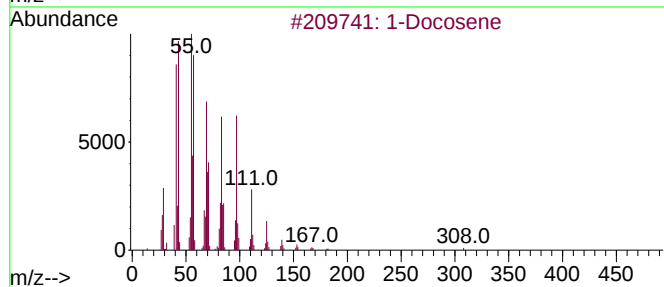
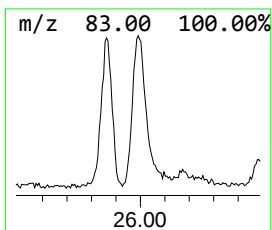
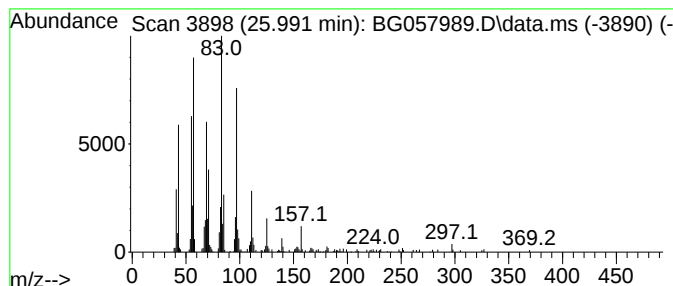
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Quant Title : SVOA CALIBRATION

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

Peak Number 18 (DEL) Alkane: Straight-Chai... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.991	7.85 ng/ul	505307	Perylene-d12	24.739

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	64
2	Triacontan-15-ol		438	C30H62O	031849-26-0	53
3	Eicosyl heptafluorobutyrate		494	C24H41F7O2	1000351-83-5	53
4	Docosyl heptafluorobutyrate		522	C26H45F7O2	1000351-83-1	53
5	1-Dotriacontanol, acetate		509	C34H68O2	023811-94-1	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
Operator : CG/JU
Sample : 03247-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DCGM5

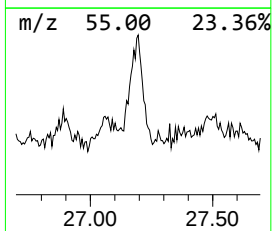
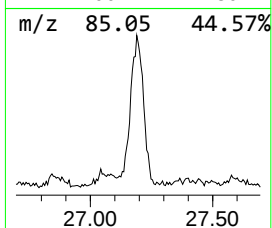
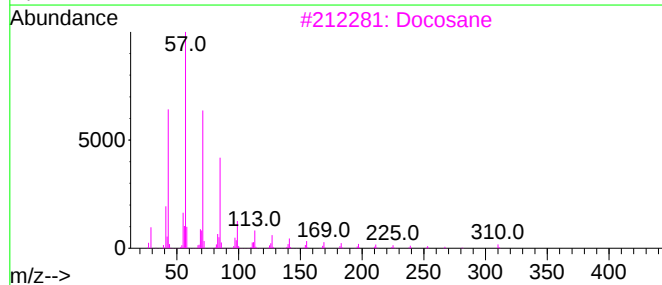
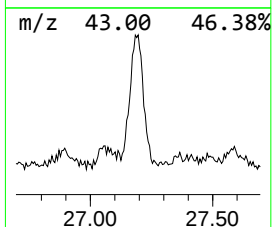
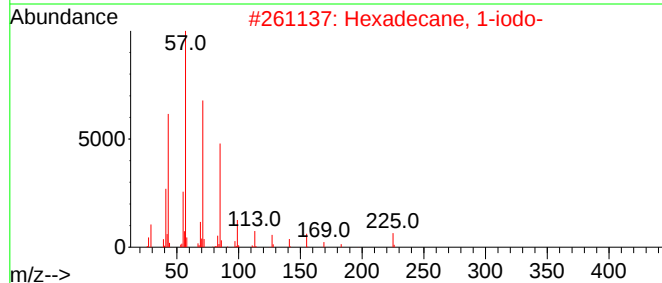
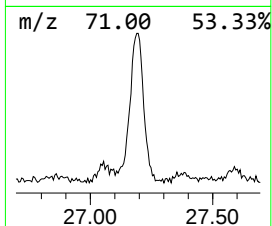
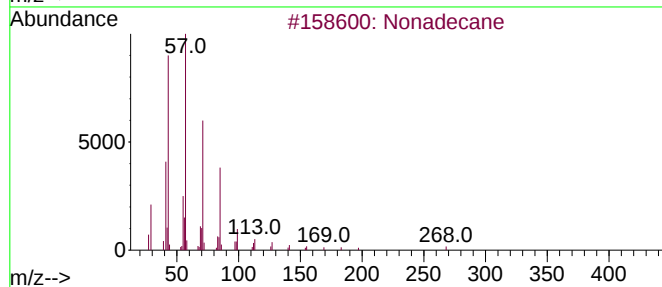
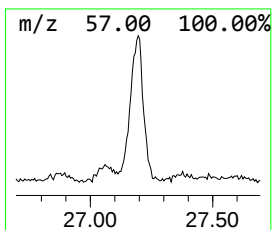
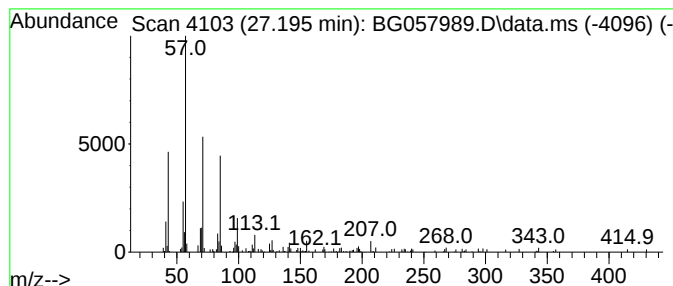
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Quant Title : SVOA CALIBRATION

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

Peak Number 19 (DEL) Alkane: Straight-Chai... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.195	4.84 ng/ul	311203	Perylene-d12	24.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83
3			Docosane	310	C22H46	000629-97-0	83
4			Tridecane, 2-methyl-	198	C14H30	001560-96-9	83
5			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
Operator : CG/JU
Sample : 03247-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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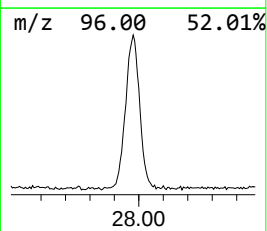
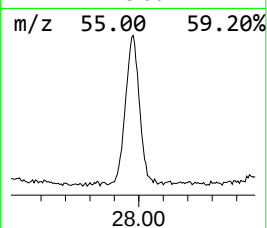
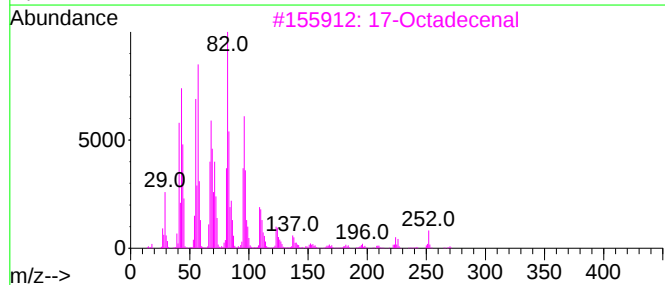
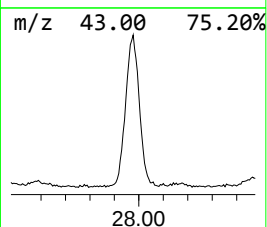
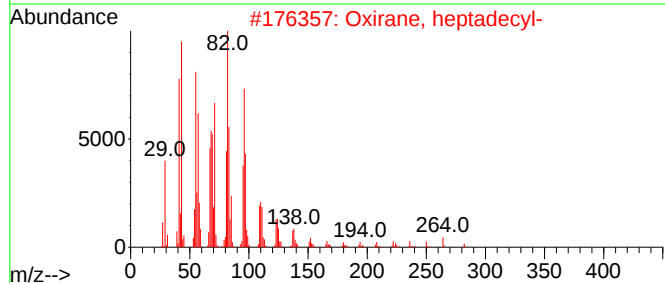
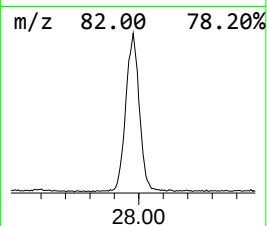
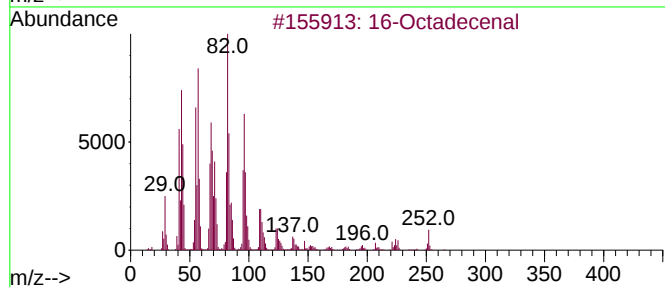
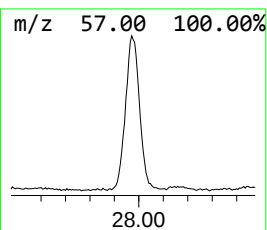
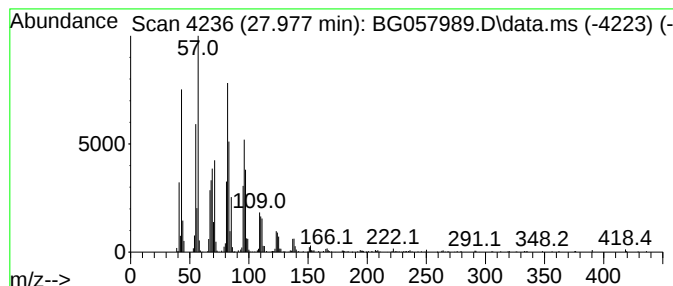
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Quant Title : SVOA CALIBRATION

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

Peak Number 20 16-Octadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.977	30.77 ng/ul	1979690	Perylene-d12	24.739

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		16-Octadecenal	266	C18H34O	056554-87-1	94
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3		17-Octadecenal	266	C18H34O	056554-86-0	91
4		Octadecanal	268	C18H36O	000638-66-4	91
5		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
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Sample : 03247-19
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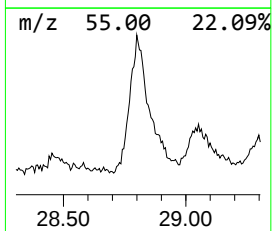
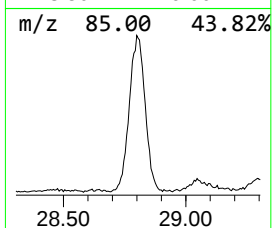
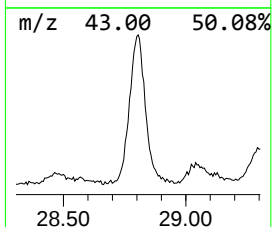
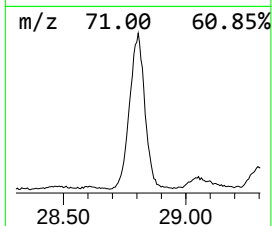
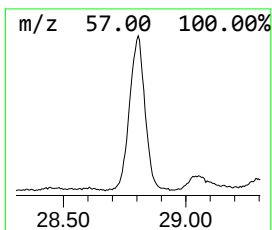
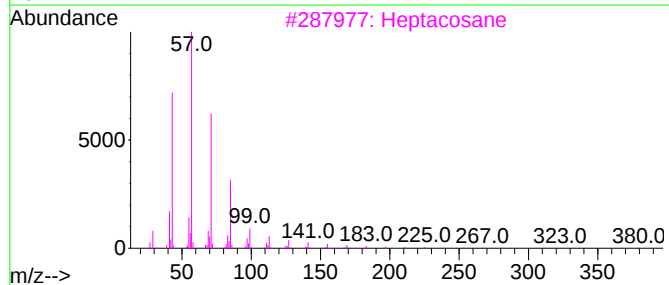
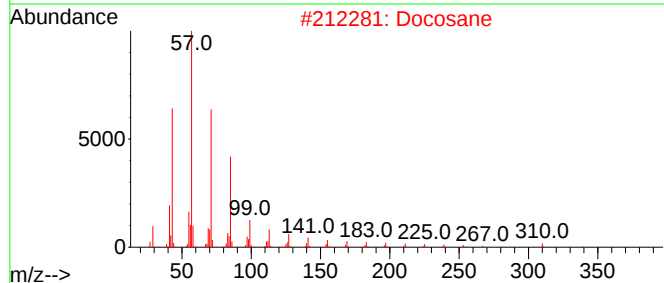
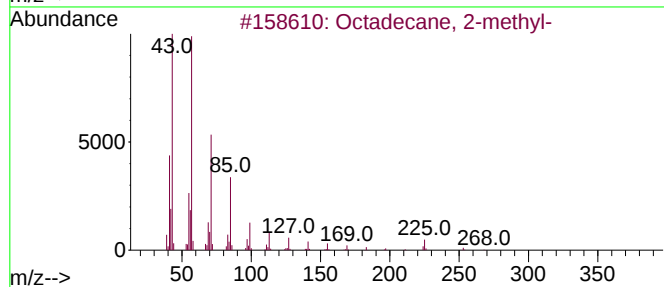
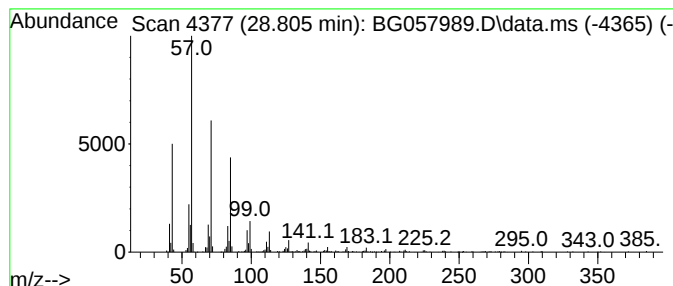
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 21 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.805	22.57 ng/ul	1452290	Perylene-d12	24.739	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2	Docosane	310	C22H46	000629-97-0	93
3	Heptacosane	380	C27H56	000593-49-7	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057989.D
Acq On : 4 Jul 2023 16:10
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Sample : 03247-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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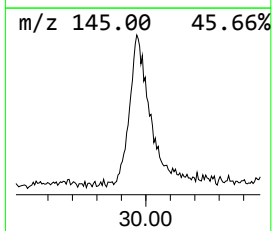
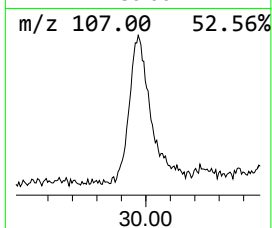
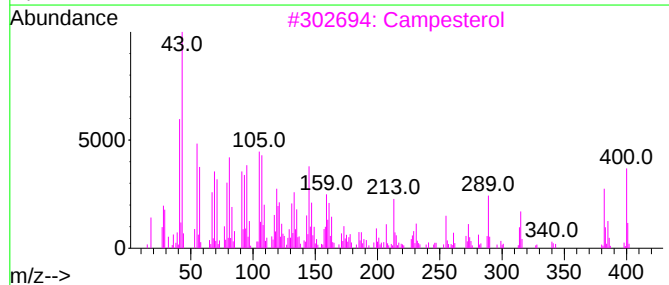
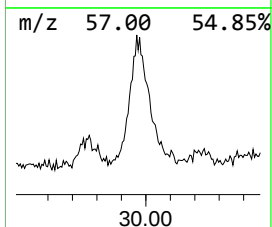
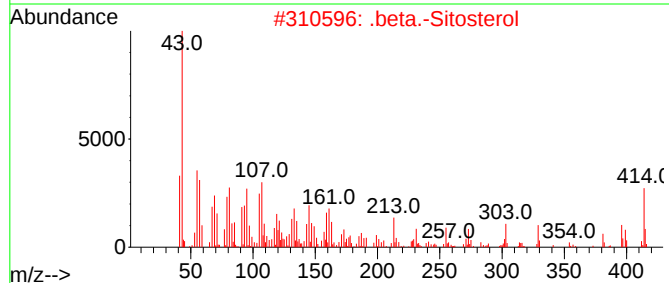
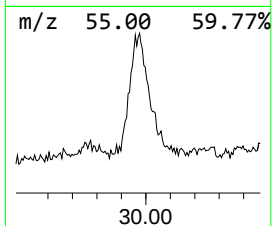
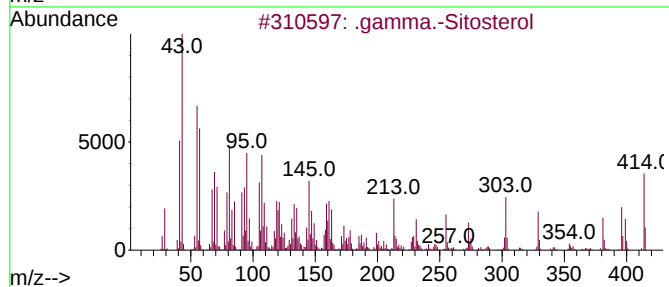
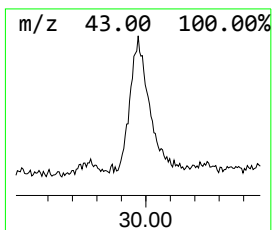
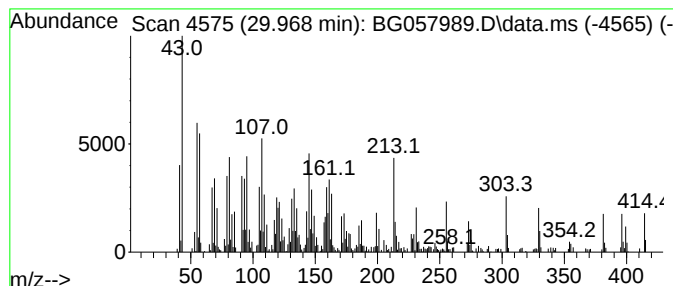
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Quant Title : SVOA CALIBRATION

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

Peak Number 22 .gamma.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.968	26.60 ng/ul	1711890	Perylene-d12	24.739

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	99
3		Campesterol	400	C28H48O	000474-62-4	53
4		.beta.-Sitosterol	414	C29H50O	000083-46-5	50
5		Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
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Operator : CG/JU
Sample : 03247-19
Misc :
ALS Vial : 47 Sample Multiplier: 1

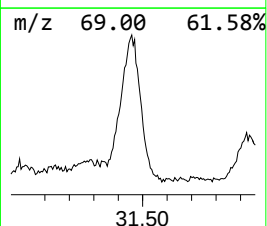
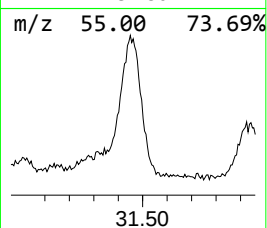
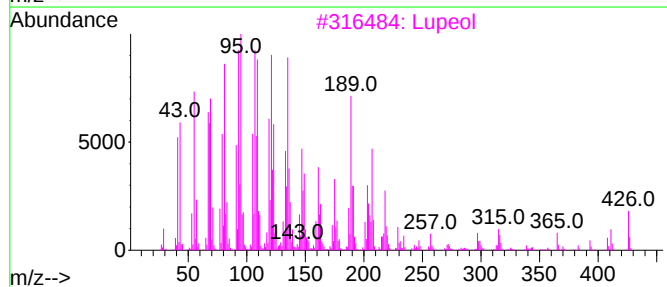
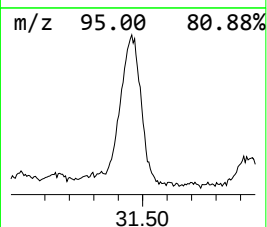
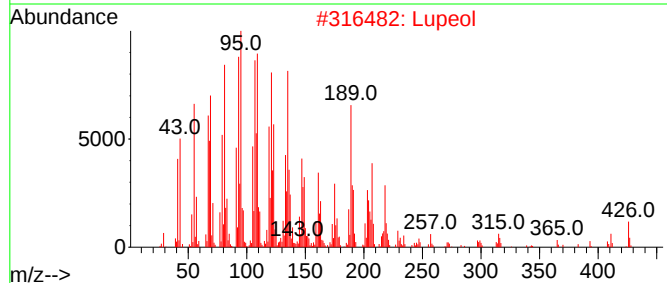
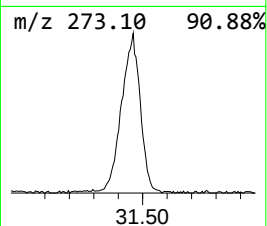
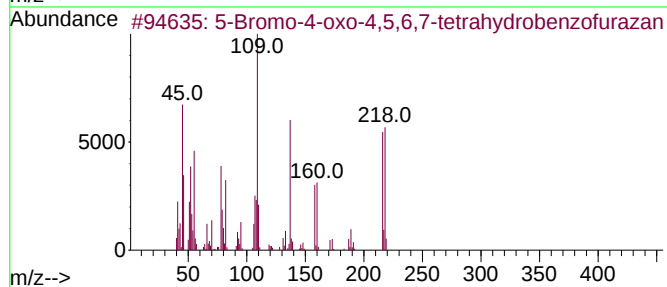
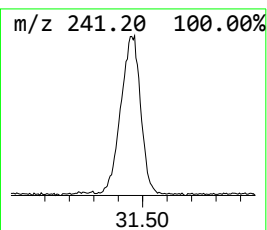
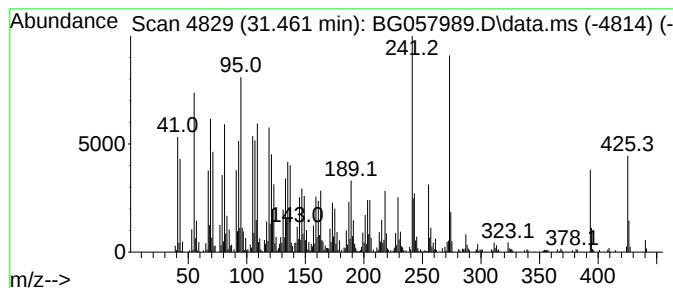
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Quant Title : SVOA CALIBRATION

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

Peak Number 23 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
31.461	59.62 ng/ul	3836300	Perylene-d12	24.739	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	90
2	Lupeol	426	C30H50O	000545-47-1	49
3	Lupeol	426	C30H50O	000545-47-1	35
4	2,6,10,15,19,23-Pentamethyl-2,6,...	446	C30H54O2	1000432-43-7	27
5	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
 Data File : BG057989.D
 Acq On : 4 Jul 2023 16:10
 Operator : CG/JU
 Sample : 03247-19
 Misc :
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DCGM5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.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
Butane, 2-metho...	3.118	140.7	ng/ul	2521200	1	7.941	358512	20.0
Disulfide, dibe...	12.195	4.3	ng/ul	129497	2	10.744	606614	20.0
Benzophenone	15.926	2.1	ng/ul	87131	3	14.575	812649	20.0
(3aR,4R,7R)-1,4...	17.019	2.7	ng/ul	130339	4	17.319	962056	20.0
n-Hexadecanoic ...	18.200	11.9	ng/ul	571951	4	17.319	962056	20.0
Octadecanoic acid	19.475	3.2	ng/ul	163735	5	21.572	1012080	20.0
3,5-di-tert-But...	19.857	5.7	ng/ul	286652	5	21.572	1012080	20.0
(DEL) Alkane: C...	20.227	2.6	ng/ul	129904	5	21.572	1012080	20.0
(DEL) Alkane: C...	21.214	11.4	ng/ul	574315	5	21.572	1012080	20.0
4,5-Dihydroxyox...	21.984	7.9	ng/ul	399041	5	21.572	1012080	20.0
(DEL) Alkane: S...	22.377	20.5	ng/ul	1038010	5	21.572	1012080	20.0
Sulfurous acid,...	23.024	4.3	ng/ul	219206	5	21.572	1012080	20.0
Octadecanal	23.376	4.9	ng/ul	317258	6	24.739	1286920	20.0
(DEL) Alkane: S...	23.823	30.1	ng/ul	1934700	6	24.739	1286920	20.0
(DEL) Alkane: S...	23.887	4.8	ng/ul	310235	6	24.739	1286920	20.0
1,19-Eicosadiene	25.262	10.3	ng/ul	665587	6	24.739	1286920	20.0
(DEL) Alkane: S...	25.861	31.5	ng/ul	2027870	6	24.739	1286920	20.0
(DEL) Alkane: S...	25.991	7.8	ng/ul	505307	6	24.739	1286920	20.0
(DEL) Alkane: S...	27.195	4.8	ng/ul	311203	6	24.739	1286920	20.0
16-Octadecenal	27.977	30.8	ng/ul	1979690	6	24.739	1286920	20.0
(DEL) Alkane: S...	28.805	22.6	ng/ul	1452290	6	24.739	1286920	20.0
.gamma.-Sitosterol	29.968	26.6	ng/ul	1711890	6	24.739	1286920	20.0
5-Bromo-4-oxo-4...	31.461	59.6	ng/ul	3836300	6	24.739	1286920	20.0