

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
 Data File : BG057954.D
 Acq On : 3 Jul 2023 14:10
 Operator : CG/JU
 Sample : 03246-12
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DCGJ9

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: BG057954.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.269	29	31	33	rBV3	1621	1741	0.14%	0.012%
2	3.375	45	49	57	rVB3	10261	16082	1.28%	0.107%
3	3.780	113	118	132	rBV	95844	159066	12.64%	1.060%
4	3.892	132	137	143	rVB6	6703	11661	0.93%	0.078%
5	4.021	154	159	164	rVB	10683	17504	1.39%	0.117%
6	4.121	173	176	180	rVB3	1967	2931	0.23%	0.020%
7	4.338	212	213	219	rVB4	1357	1740	0.14%	0.012%
8	4.485	236	238	243	rVB3	1927	1908	0.15%	0.013%
9	4.761	284	285	291	rBV4	1425	2416	0.19%	0.016%
10	4.932	307	314	317	rVB3	1520	2856	0.23%	0.019%
11	5.026	327	330	335	rBV3	2868	4378	0.35%	0.029%
12	5.126	342	347	350	rVB3	1443	2310	0.18%	0.015%
13	5.155	350	352	356	rBV3	1542	2255	0.18%	0.015%
14	6.495	576	580	584	rBV4	1161	1930	0.15%	0.013%
15	6.923	648	653	654	rBV3	2076	2365	0.19%	0.016%
16	7.094	675	682	693	rVB	136684	234316	18.62%	1.561%
17	7.258	704	710	720	rBV	113366	183159	14.55%	1.220%
18	7.464	738	745	754	rBV	133420	223325	17.75%	1.488%
19	7.558	759	761	764	rVB4	2018	2000	0.16%	0.013%
20	7.934	818	825	832	rBV	130740	214980	17.08%	1.432%
21	8.639	938	945	951	rBV2	159375	277656	22.06%	1.850%
22	8.698	951	955	961	rVV3	10347	17010	1.35%	0.113%
23	8.757	964	965	972	rVB2	1064	1513	0.12%	0.010%
24	9.097	1016	1023	1031	rVB	133598	236820	18.82%	1.578%
25	9.814	1138	1145	1153	rBV	102623	184286	14.64%	1.228%
26	10.361	1231	1238	1248	rBV	169930	299086	23.76%	1.993%
27	10.513	1261	1264	1266	rBV2	1410	1704	0.14%	0.011%
28	10.737	1295	1302	1311	rBV	200170	348107	27.66%	2.319%
29	10.872	1318	1325	1343	rVB	149121	276987	22.01%	1.846%
30	12.211	1548	1553	1558	rVB3	1814	2932	0.23%	0.020%
31	12.323	1567	1572	1578	rBV3	2713	3829	0.30%	0.026%
32	12.546	1604	1610	1614	rBV2	1364	2172	0.17%	0.014%
33	12.922	1670	1674	1680	rVB3	2401	2984	0.24%	0.020%
34	13.169	1712	1716	1721	rBV3	2933	4329	0.34%	0.029%
35	13.392	1748	1754	1756	rBV2	1549	2072	0.16%	0.014%
36	13.457	1761	1765	1770	rVB2	9411	12657	1.01%	0.084%

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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
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37	13.974	1846	1853	1863	rBV	363897	525107	41.72%	3.499%
38	14.262	1895	1902	1915	rVB2	397807	642586	51.06%	4.281%
39	14.456	1933	1935	1939	rVB2	2034	2532	0.20%	0.017%
40	14.567	1948	1954	1964	rVB	349296	537644	42.72%	3.582%
41	14.761	1980	1987	2001	rBV	148111	245108	19.48%	1.633%
42	14.914	2010	2013	2018	rBV3	2071	2711	0.22%	0.018%
43	14.979	2020	2024	2033	rBV2	8203	14032	1.11%	0.093%
44	15.408	2094	2097	2100	rVB2	2461	2569	0.20%	0.017%
45	15.560	2116	2123	2131	rBV	574178	863900	68.64%	5.756%
46	15.672	2136	2142	2151	rBV	163482	233871	18.58%	1.558%
47	15.919	2179	2184	2190	rBV	150812	221300	17.58%	1.474%
48	15.966	2190	2192	2196	rVB4	2033	2195	0.17%	0.015%
49	16.271	2239	2244	2247	rBV3	1424	2096	0.17%	0.014%
50	16.483	2276	2280	2286	rVB2	7169	10600	0.84%	0.071%
51	16.706	2315	2318	2328	rVB5	2557	5433	0.43%	0.036%
52	16.841	2339	2341	2345	rVB3	1513	1614	0.13%	0.011%
53	17.065	2376	2379	2382	rBV	2018	1749	0.14%	0.012%
54	17.211	2401	2404	2405	rBV2	2405	2450	0.19%	0.016%
55	17.223	2405	2406	2409	rVB2	4348	2472	0.20%	0.016%
56	17.270	2409	2414	2415	rBV4	2351	3563	0.28%	0.024%
57	17.311	2415	2421	2431	rVV	506061	753396	59.86%	5.020%
58	17.411	2431	2438	2447	rVB2	622486	947115	75.26%	6.310%
59	17.493	2447	2452	2456	rBV5	9567	12959	1.03%	0.086%
60	17.593	2467	2469	2475	rVB7	1965	1645	0.13%	0.011%
61	17.687	2481	2485	2487	rBV3	3326	3635	0.29%	0.024%
62	17.758	2495	2497	2500	rVB2	2081	1745	0.14%	0.012%
63	17.793	2500	2503	2504	rBV2	2362	2030	0.16%	0.014%
64	17.975	2532	2534	2539	rVB6	2167	2293	0.18%	0.015%
65	18.081	2547	2552	2553	rBV5	3530	4931	0.39%	0.033%
66	18.146	2561	2563	2566	rVB3	2301	2005	0.16%	0.013%
67	18.199	2566	2572	2581	rBV	199295	311042	24.71%	2.072%
68	18.369	2599	2601	2602	rBV2	3076	2168	0.17%	0.014%
69	18.622	2642	2644	2647	rBV4	3794	4712	0.37%	0.031%
70	18.768	2667	2669	2670	rBV2	3681	2484	0.20%	0.017%
71	18.857	2681	2684	2685	rBV3	5609	5317	0.42%	0.035%
72	19.050	2714	2717	2720	rBV5	9860	11778	0.94%	0.078%
73	19.092	2721	2724	2732	rVB7	21272	30549	2.43%	0.204%
74	19.256	2746	2752	2758	rVB8	12822	29045	2.31%	0.194%
75	19.332	2760	2765	2766	rBV4	19249	25019	1.99%	0.167%
76	19.362	2766	2770	2777	rVB2	32078	57541	4.57%	0.383%

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 Title : SVOA CALIBRATION

77	19.468	2784	2788	2799	rVB	53351	88181	7.01%	0.588%
78	19.620	2810	2814	2818	rBV6	7197	9762	0.78%	0.065%
79	19.697	2821	2827	2836	rBV	862353	1258520	100.00%	8.385%
80	20.226	2914	2917	2921	rVB3	18369	22656	1.80%	0.151%
81	20.719	2996	3001	3004	rBV2	37931	63077	5.01%	0.420%
82	21.213	3080	3085	3088	rBV	173376	305927	24.31%	2.038%
83	21.283	3090	3097	3099	rVV6	109532	271109	21.54%	1.806%
84	21.565	3138	3145	3151	rBV2	461131	758044	60.23%	5.051%
85	21.759	3162	3178	3179	rBV3	365752	1179788	93.74%	7.861%
86	22.347	3275	3278	3288	rBV5	36754	84452	6.71%	0.563%
87	23.028	3389	3394	3399	rBV2	37402	67948	5.40%	0.453%
88	23.815	3523	3528	3534	rVB2	56918	113948	9.05%	0.759%
89	24.509	3637	3646	3657	rVB2	431639	1224554	97.30%	8.159%
90	24.726	3673	3683	3698	rBV	312822	943223	74.95%	6.285%
91	25.860	3869	3876	3886	rVB3	61107	174802	13.89%	1.165%
92	27.188	4095	4102	4114	rVB2	43836	144653	11.49%	0.964%

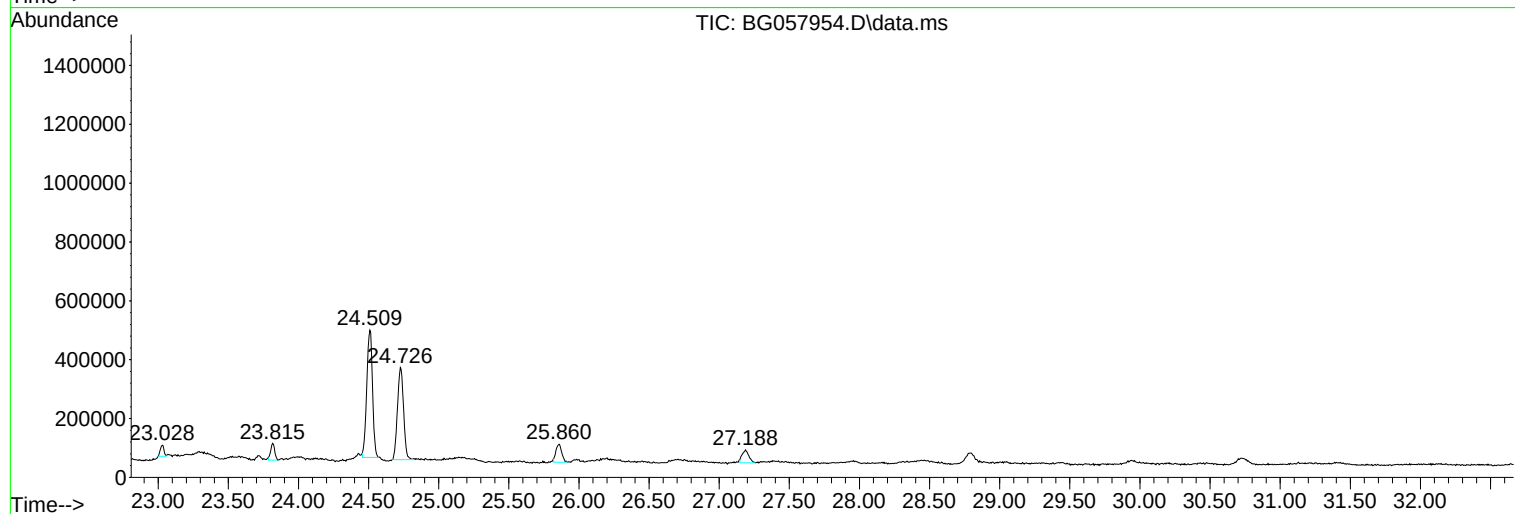
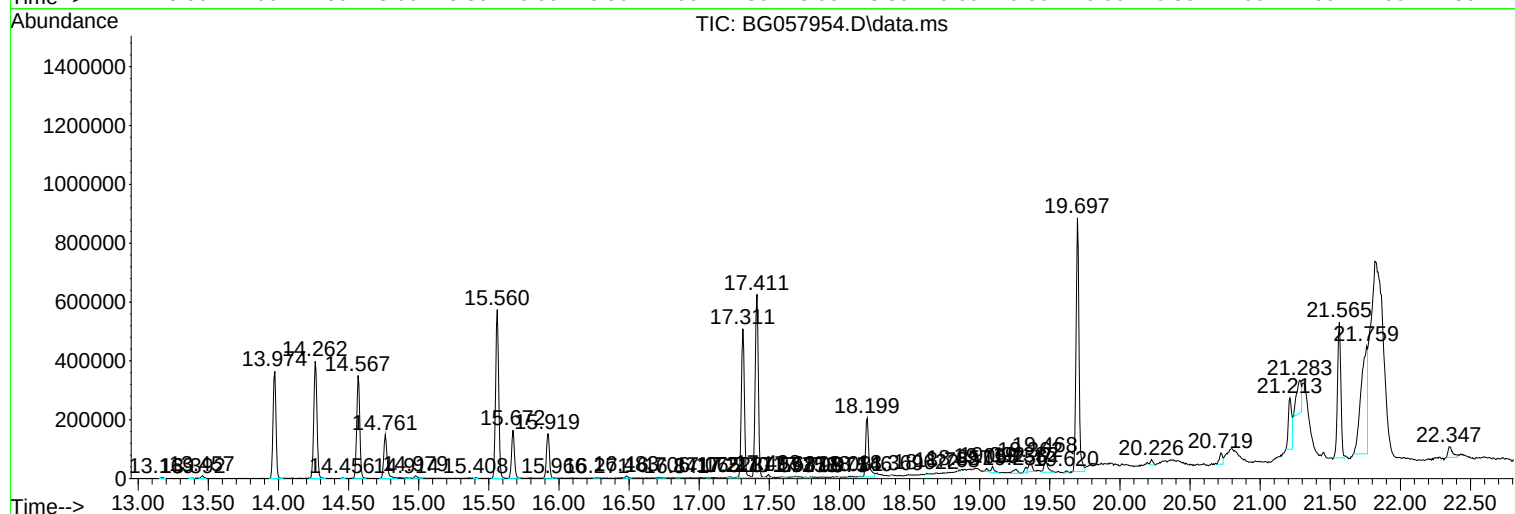
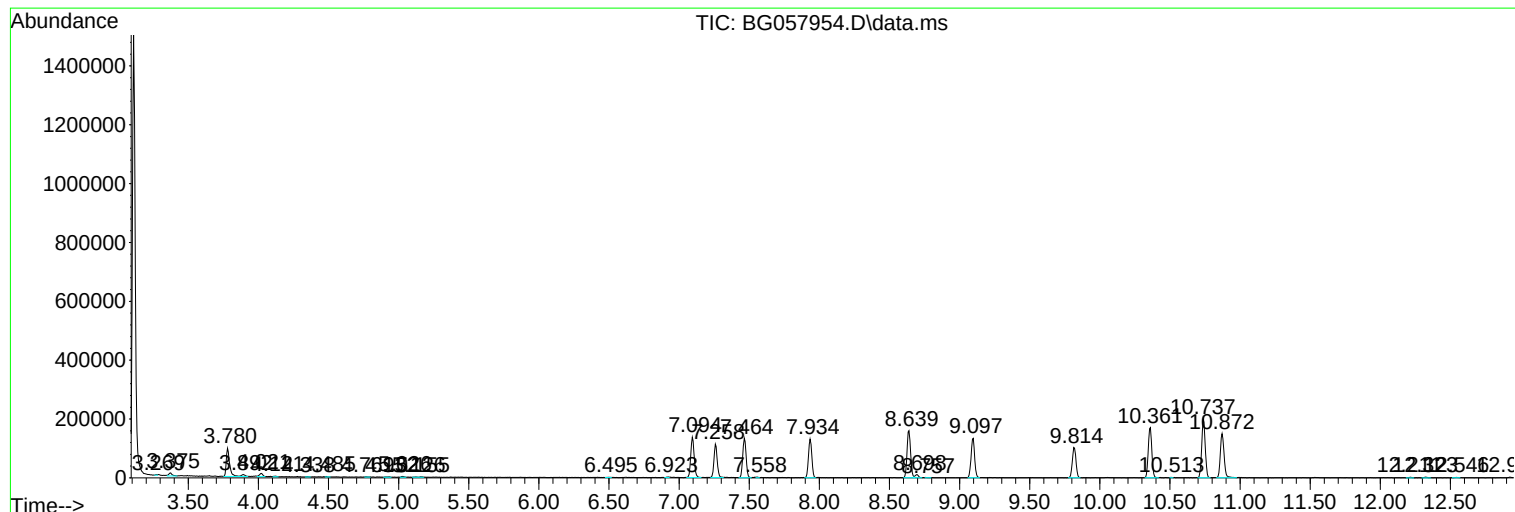
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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



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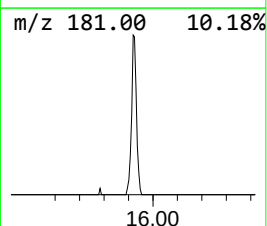
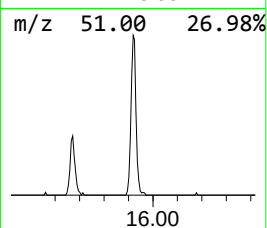
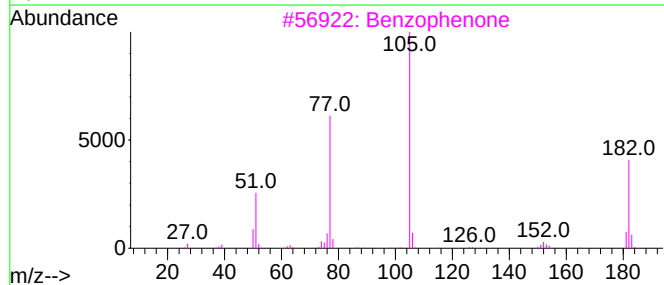
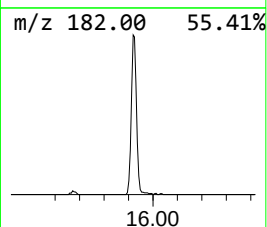
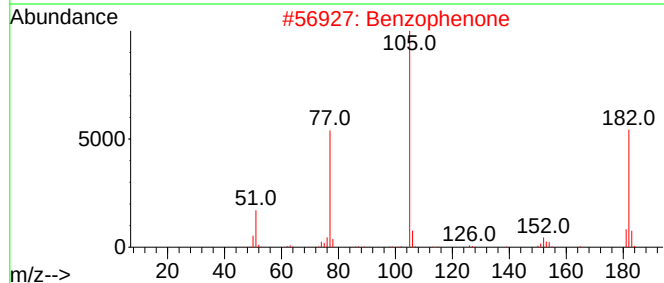
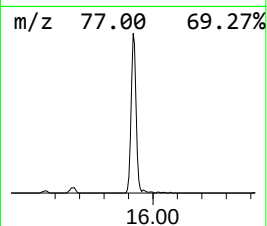
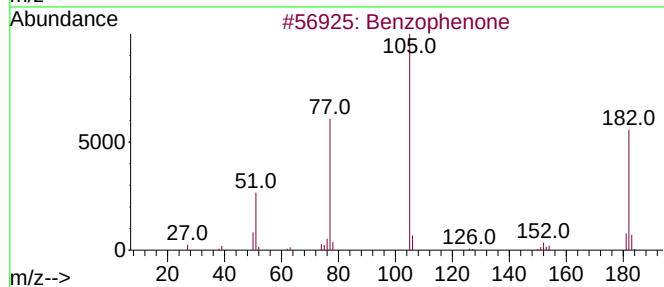
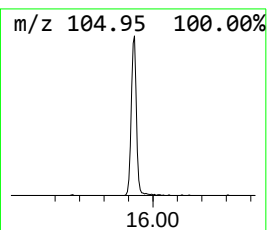
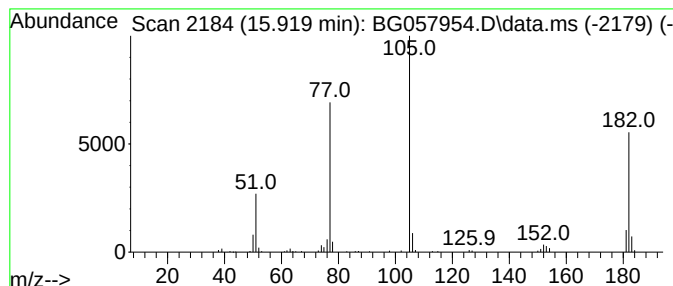
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.919	8.23 ng/ul	221300	Acenaphthene-d10	14.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzophenone	182	C13H10O	000119-61-9	95
3			Benzophenone	182	C13H10O	000119-61-9	94
4			Benzophenone	182	C13H10O	000119-61-9	90
5			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	53



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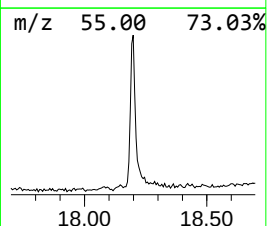
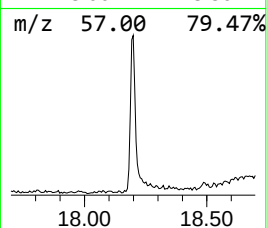
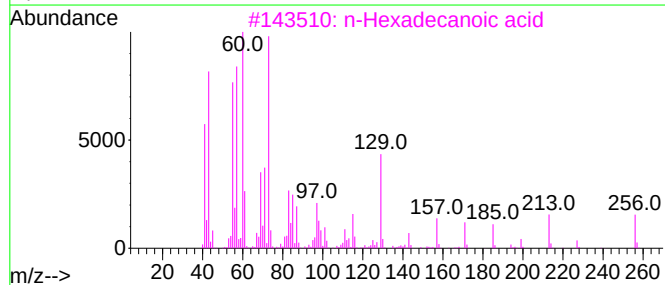
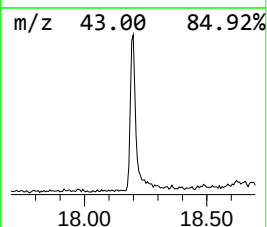
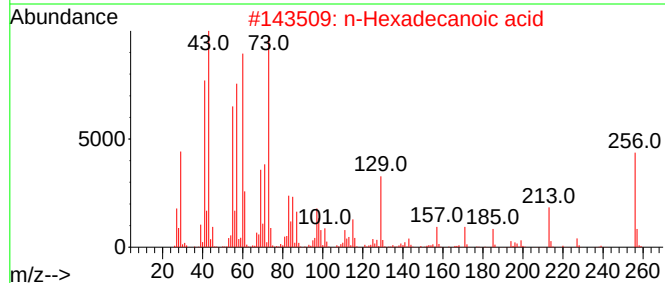
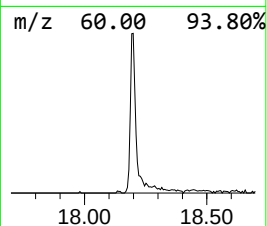
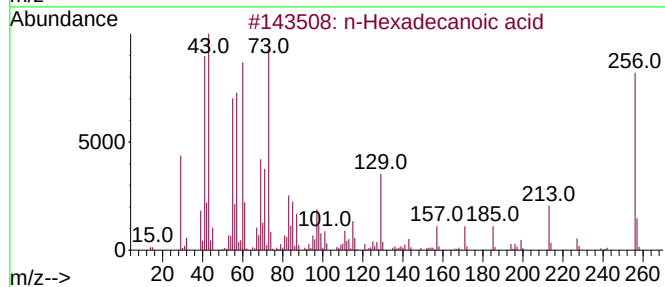
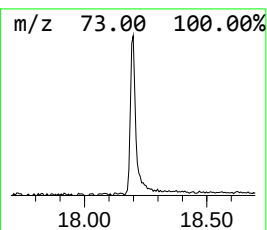
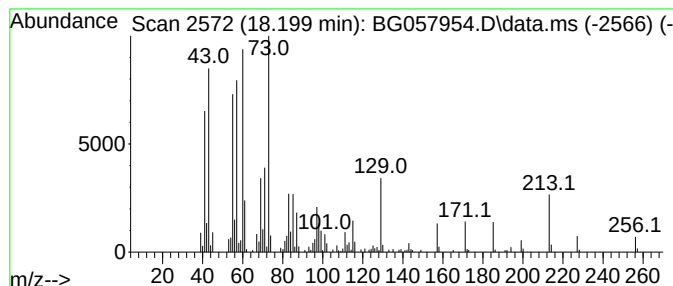
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	8.26 ng/ul	311042	Phenanthrene-d10	17.311

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	93
5			Tridecanoic acid	214	C13H26O2	000638-53-9	89



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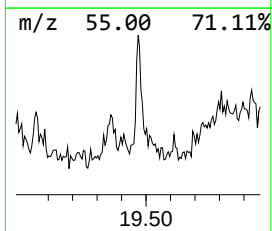
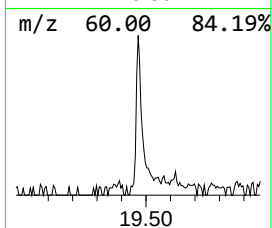
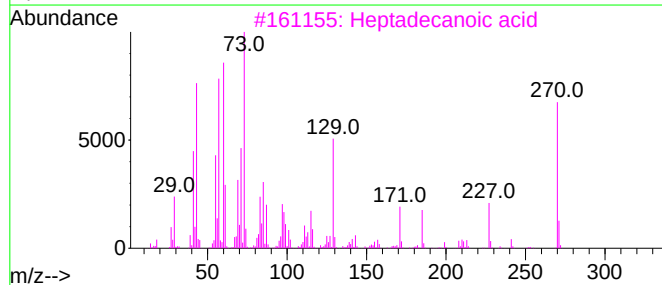
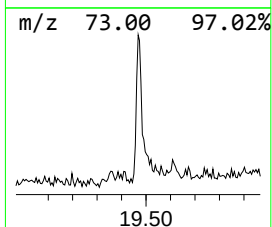
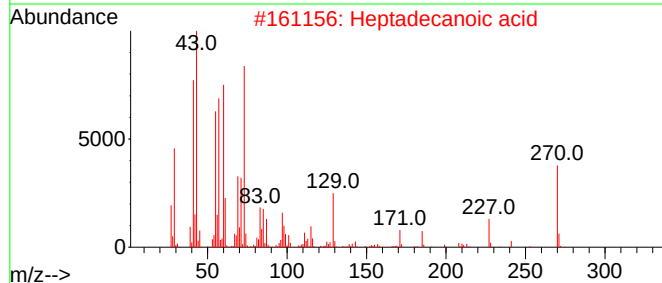
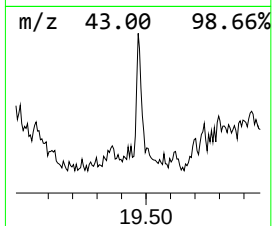
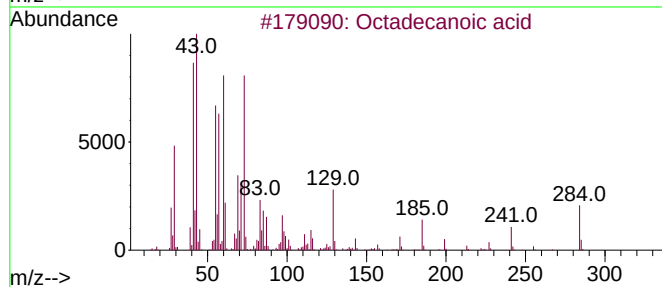
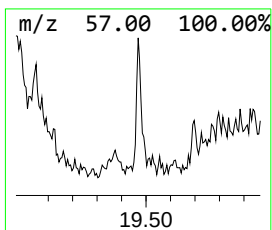
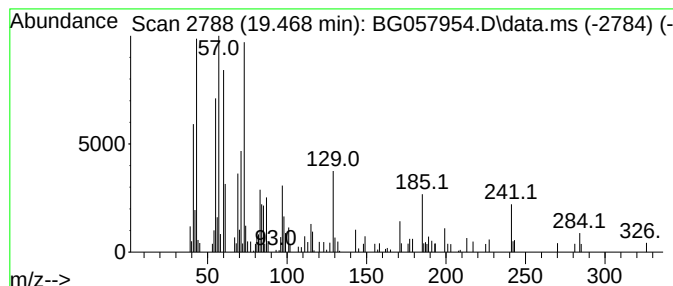
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.468	2.33 ng/ul	88181	Chrysene-d12	21.565

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Heptadecanoic acid	270	C17H34O2	000506-12-7	89
3			Heptadecanoic acid	270	C17H34O2	000506-12-7	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			Octadecanoic acid	284	C18H36O2	000057-11-4	72



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ClientSampleId :
DCGJ9

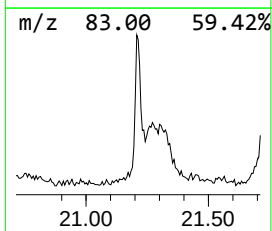
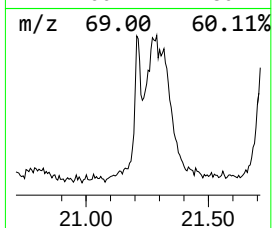
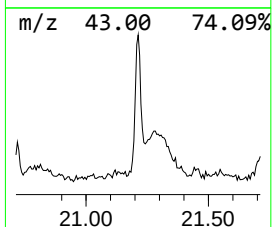
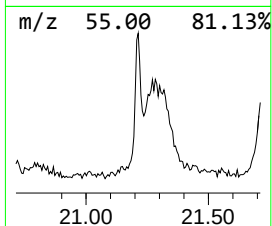
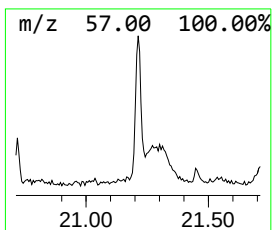
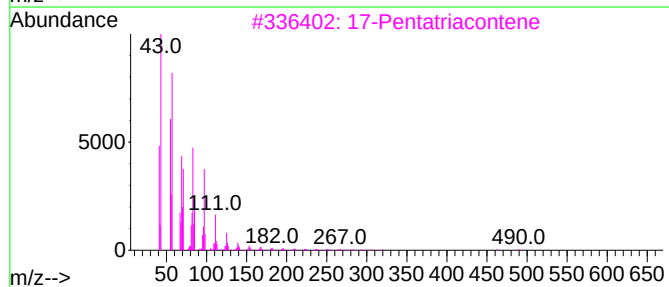
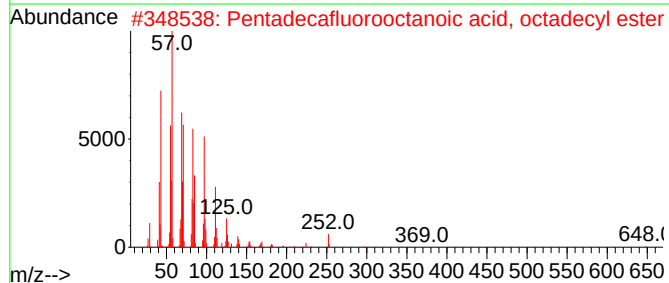
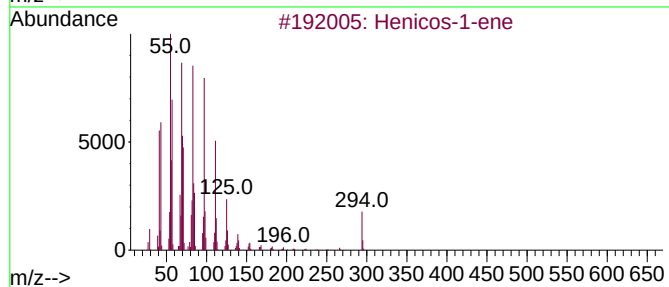
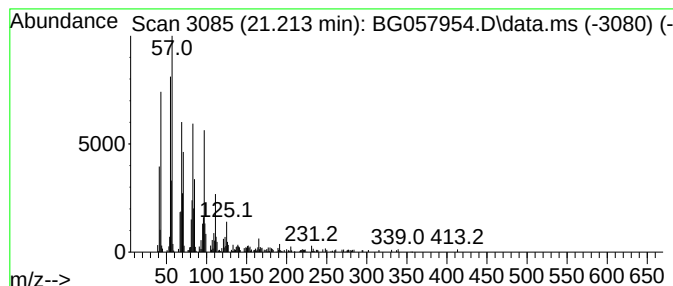
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.213	8.07 ng/ul	305927	Chrysene-d12	21.565

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Henicos-1-ene	294	C21H42	001599-68-4	96
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			17-Pentatriacontene	491	C35H70	006971-40-0	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5			Nonacos-1-ene	406	C29H58	018835-35-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057954.D
Acq On : 3 Jul 2023 14:10
Operator : CG/JU
Sample : 03246-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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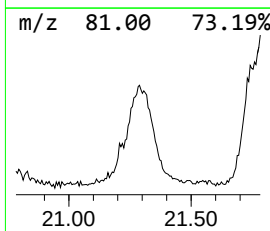
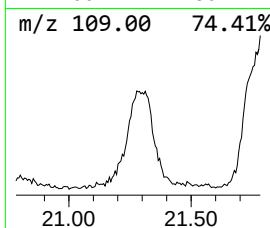
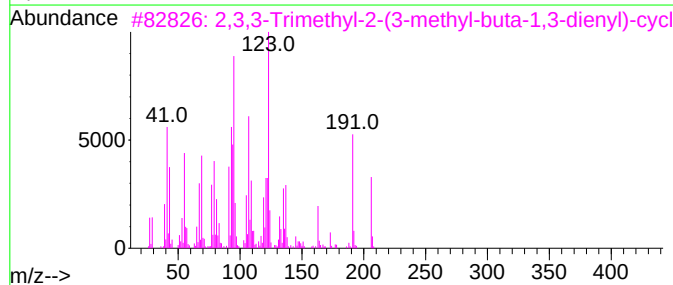
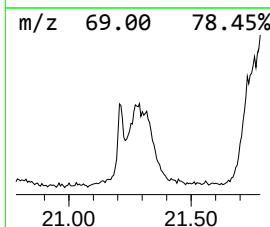
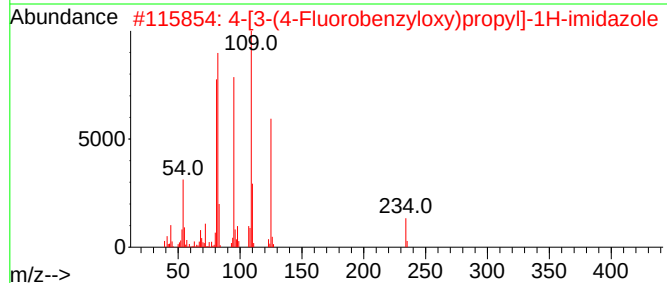
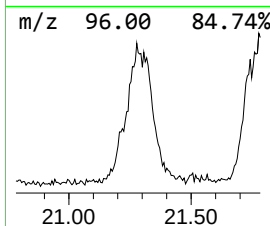
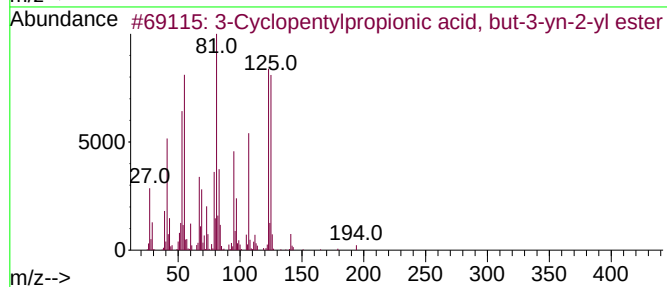
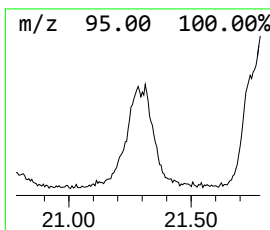
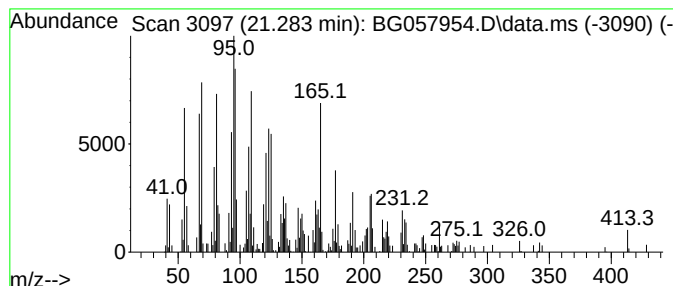
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.283	7.15 ng/ul	271109	Chrysene-d12	21.565

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Cyclopentylpropionic acid, but...	194	C12H18O2	1000292-46-4	38
2			4-[3-(4-Fluorobenzyloxy)propyl]-...	234	C13H15FN2O	1000311-87-2	38
3			2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	35
4			1H-Imidazole, 2-ethyl-	96	C5H8N2	001072-62-4	35
5			Imidazole, 4-methyl-5-[3,3,3-tri...	234	C10H13F3N2O	1000129-15-8	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
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Acq On : 3 Jul 2023 14:10
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Instrument :
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ClientSampleId :
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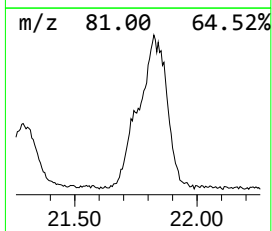
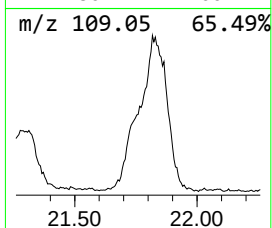
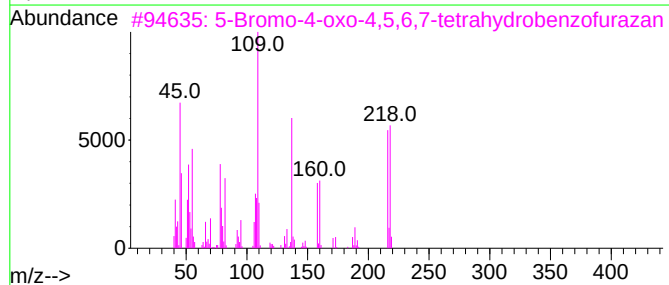
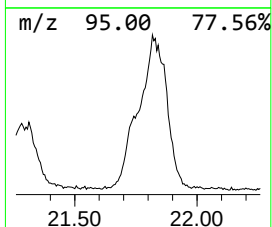
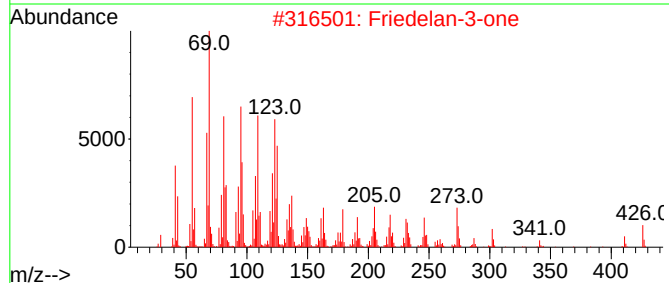
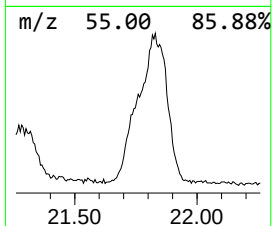
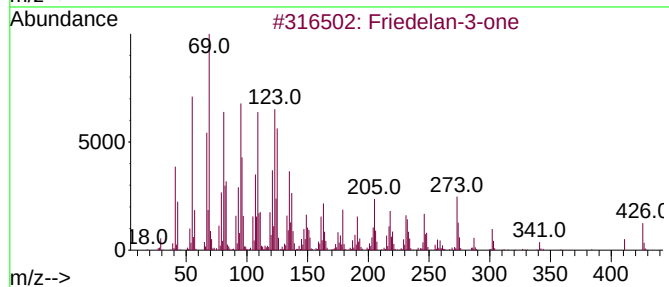
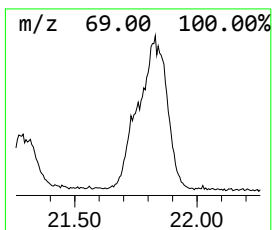
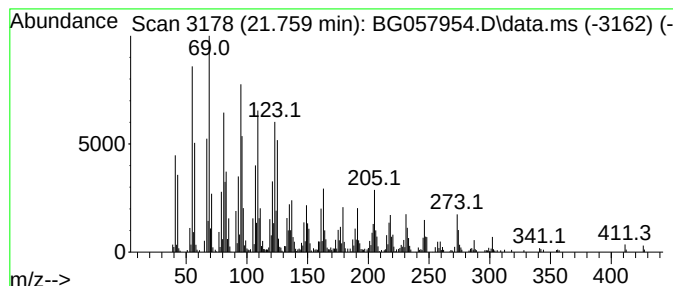
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.759	31.13 ng/ul	1179790	Chrysene-d12	21.565

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Friedelan-3-one	426	C30H50O	000559-74-0	96
2			Friedelan-3-one	426	C30H50O	000559-74-0	96
3			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	90
4			Sesquirosefuran	218	C15H22O	039007-93-7	64
5			Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
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Acq On : 3 Jul 2023 14:10
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Sample : 03246-12
Misc :
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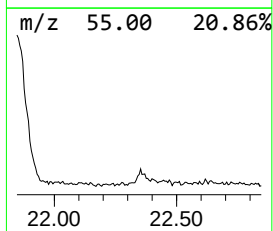
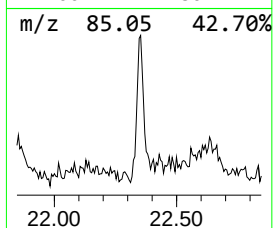
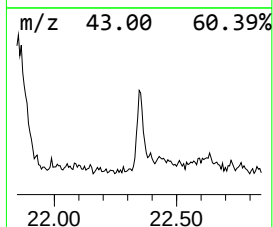
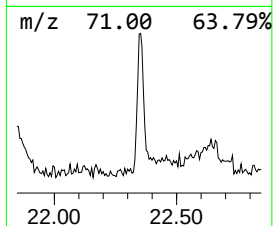
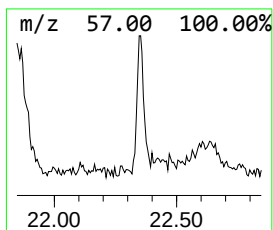
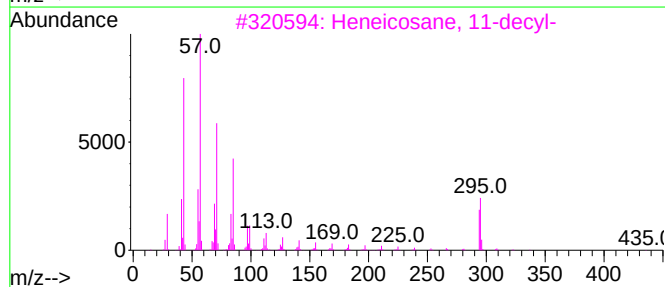
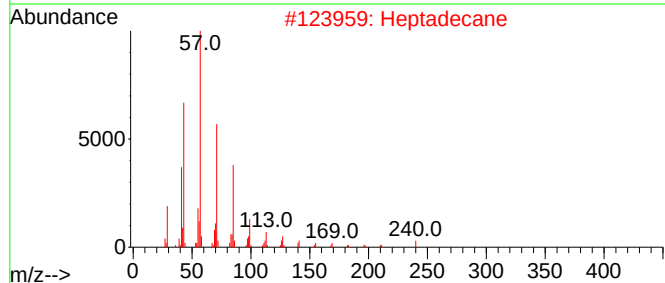
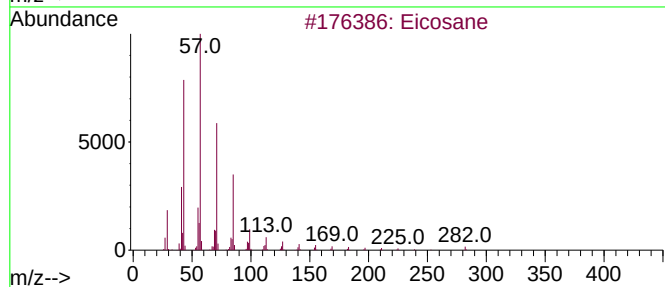
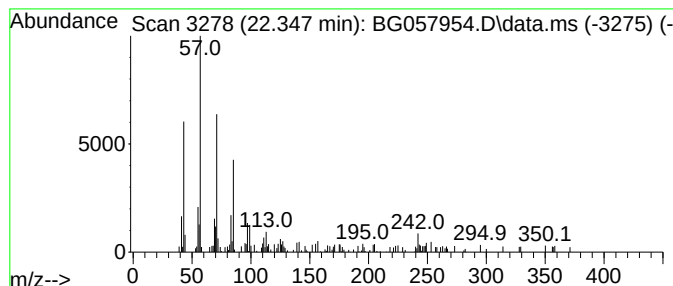
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.347	2.23 ng/ul	84452	Chrysene-d12		21.565	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Heptadecane		240	C17H36	000629-78-7	91
3	Heneicosane, 11-decyl-		437	C31H64	055320-06-4	87
4	Tetratetracontane		619	C44H90	007098-22-8	87
5	Heptadecane		240	C17H36	000629-78-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057954.D
Acq On : 3 Jul 2023 14:10
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Sample : 03246-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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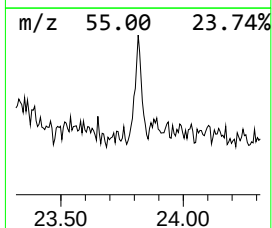
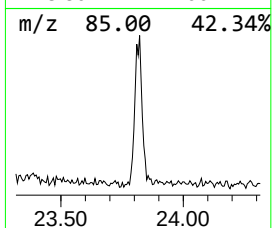
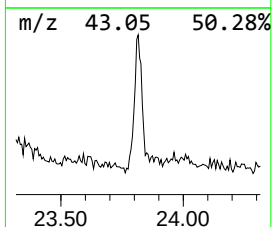
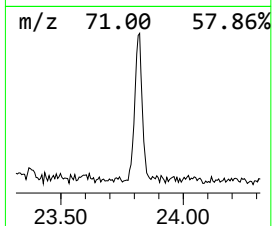
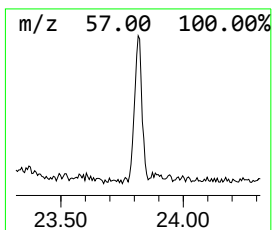
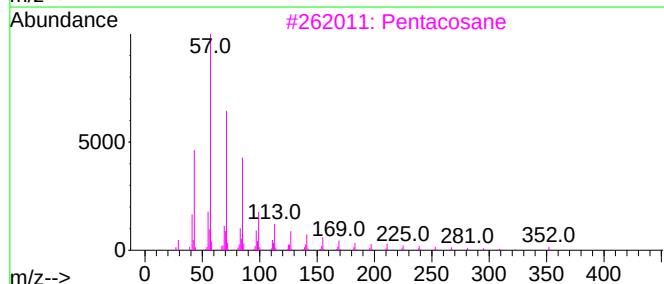
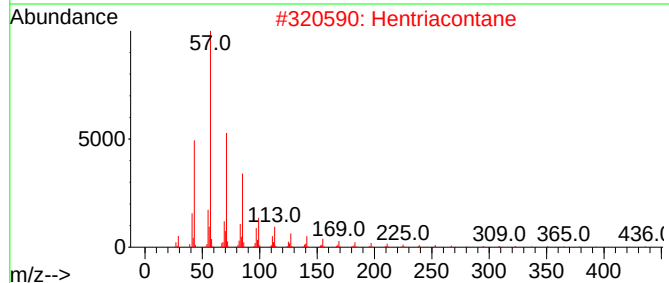
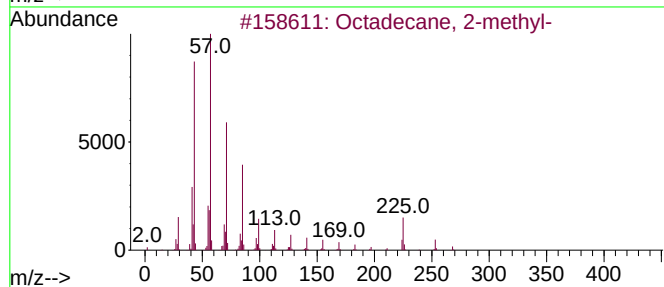
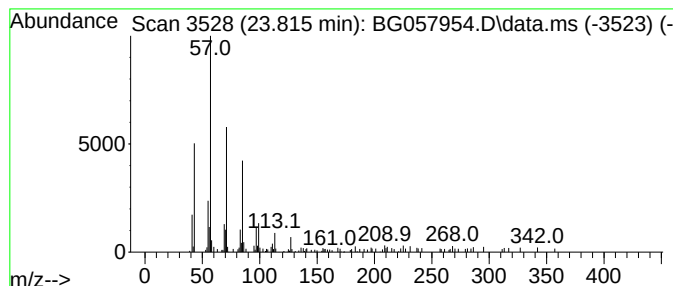
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.816	2.42 ng/ul	113948	Perylene-d12	24.726

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
2		Hentriacontane	437	C31H64	000630-04-6	87
3		Pentacosane	352	C25H52	000629-99-2	87
4		Nonadecane	268	C19H40	000629-92-5	87
5		Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057954.D
Acq On : 3 Jul 2023 14:10
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Sample : 03246-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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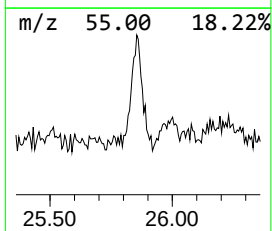
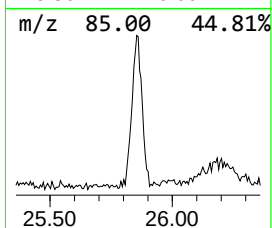
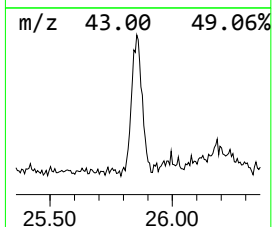
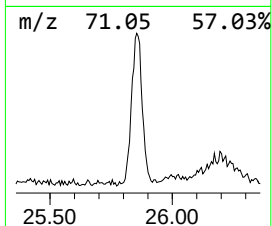
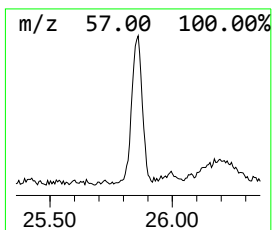
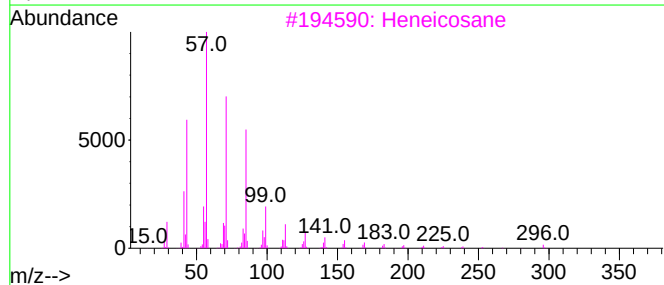
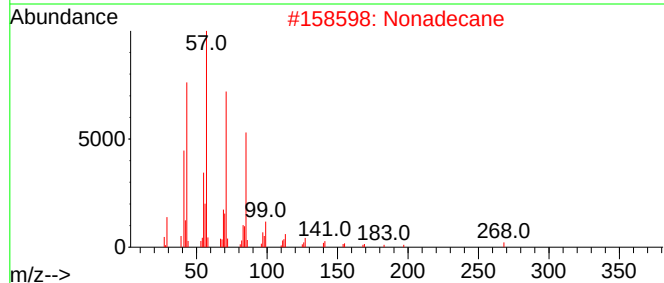
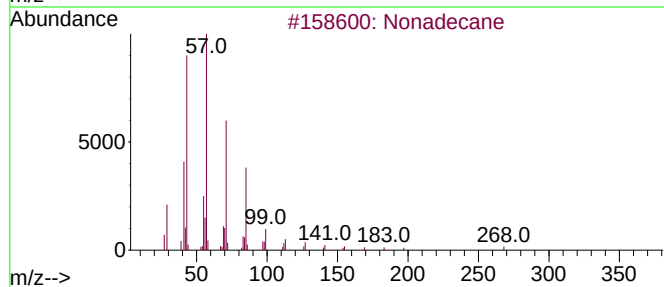
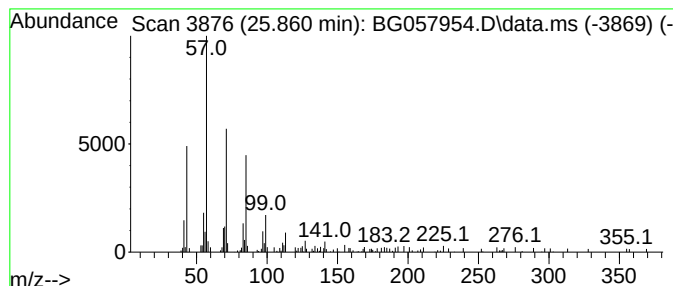
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.860	3.71 ng/ul	174802	Perylene-d12	24.726

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	93
2		Nonadecane	268	C19H40	000629-92-5	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Heneicosane	296	C21H44	000629-94-7	87
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
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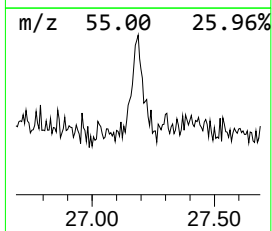
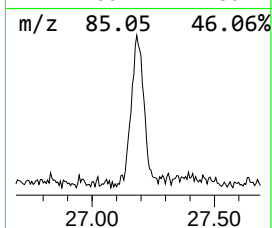
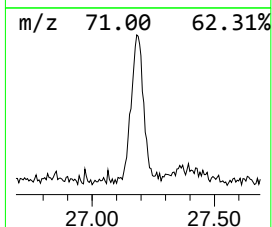
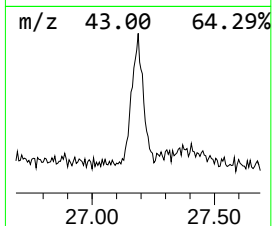
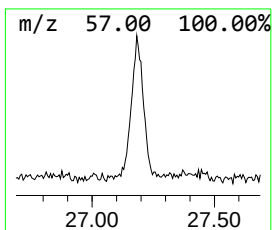
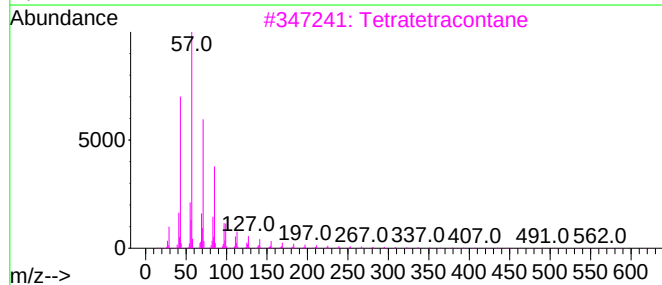
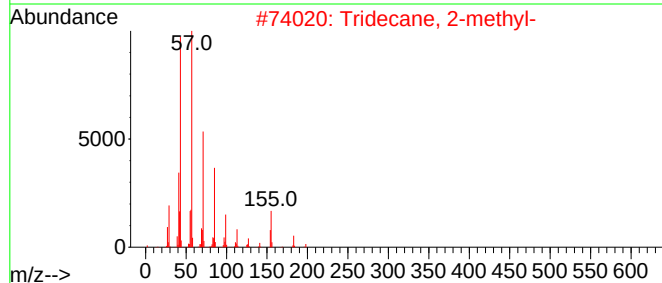
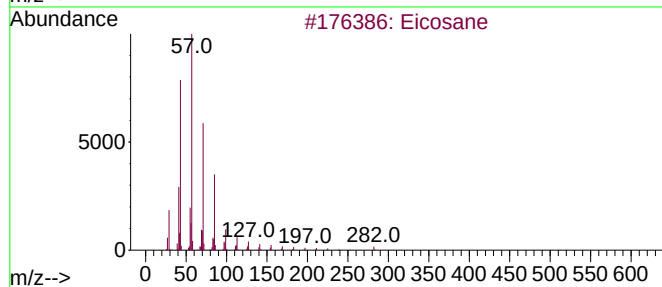
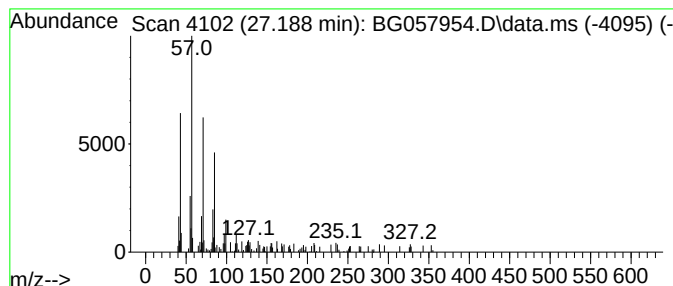
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.188	3.07 ng/ul	144653	Perylene-d12	24.726

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	83
2		Tridecane, 2-methyl-	198	C14H30	001560-96-9	64
3		Tetratetracontane	619	C44H90	007098-22-8	64
4		Tetradecane	198	C14H30	000629-59-4	53
5		Tetradecane	198	C14H30	000629-59-4	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057954.D
Acq On : 3 Jul 2023 14:10
Operator : CG/JU
Sample : 03246-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGJ9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.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
Benzophenone	15.919	8.2	ng/ul	221300	3	14.568	537644	20.0
n-Hexadecanoic ...	18.198	8.3	ng/ul	311042	4	17.311	753396	20.0
Octadecanoic acid	19.468	2.3	ng/ul	88181	5	21.565	758044	20.0
(DEL) Alkane: S...	21.213	8.1	ng/ul	305927	5	21.565	758044	20.0
unknown-01	21.283	7.2	ng/ul	271109	5	21.565	758044	20.0
5-Bromo-4-oxo-4...	21.759	31.1	ng/ul	1179790	5	21.565	758044	20.0
(DEL) Alkane: S...	22.347	2.2	ng/ul	84452	5	21.565	758044	20.0
(DEL) Alkane: S...	23.816	2.4	ng/ul	113948	6	24.726	943223	20.0
(DEL) Alkane: S...	25.860	3.7	ng/ul	174802	6	24.726	943223	20.0
(DEL) Alkane: S...	27.188	3.1	ng/ul	144653	6	24.726	943223	20.0