

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011023\
 Data File : BG056239.D
 Acq On : 10 Jan 2023 11:38
 Operator : CG/JU
 Sample : PB150093BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SBLK093

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-BG010423.M
 Title : SVOA CALIBRATION

Signal : TIC: BG056239.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.358	7	12	18	rVB	22280	36861	2.06%	0.205%
2	3.470	29	31	33	rBV3	2632	2290	0.13%	0.013%
3	3.628	52	58	67	rVB2	11885	19873	1.11%	0.110%
4	3.881	99	101	105	rVB3	1921	1984	0.11%	0.011%
5	4.063	128	132	148	rBV	120908	220396	12.29%	1.224%
6	4.422	189	193	199	rVB	9429	13961	0.78%	0.078%
7	7.459	702	710	719	rBV	182576	320095	17.85%	1.777%
8	7.635	732	740	754	rVB	159501	259859	14.49%	1.443%
9	7.853	770	777	787	rVB	187182	322677	17.99%	1.792%
10	8.329	849	858	866	rBV	175089	305358	17.03%	1.695%
11	9.022	967	976	988	rBV	245941	440294	24.55%	2.445%
12	9.504	1050	1058	1070	rVB	170671	310530	17.32%	1.724%
13	10.232	1174	1182	1189	rBV	149278	276939	15.44%	1.538%
14	10.767	1264	1273	1285	rBV	273167	496991	27.71%	2.759%
15	11.161	1331	1340	1348	rBV	253622	454722	25.36%	2.525%
16	11.284	1354	1361	1370	rBV	235686	436229	24.33%	2.422%
17	12.724	1601	1606	1616	rBB2	6363	8970	0.50%	0.050%
18	14.328	1872	1879	1886	rBV	544092	801744	44.71%	4.452%
19	14.639	1925	1932	1941	rVB	652108	998500	55.68%	5.544%
20	14.944	1976	1984	1993	rVB	482133	759571	42.36%	4.217%
21	15.103	2005	2011	2023	rBV	178283	294357	16.41%	1.634%
22	15.926	2144	2151	2160	rVB	854337	1323033	73.77%	7.346%
23	16.031	2162	2169	2181	rVB	202300	301358	16.80%	1.673%
24	16.161	2187	2191	2198	rVB2	3380	5338	0.30%	0.030%
25	17.677	2442	2449	2457	rBV	660527	990056	55.21%	5.497%
26	17.776	2459	2466	2473	rBV	951675	1451468	80.94%	8.059%
27	19.380	2737	2739	2742	rBV2	1862	2357	0.13%	0.013%
28	19.492	2752	2758	2759	rBV3	2080	3877	0.22%	0.022%
29	19.610	2773	2778	2783	rBV2	17132	21385	1.19%	0.119%
30	19.674	2785	2789	2796	rVB	12485	19823	1.11%	0.110%
31	19.921	2828	2831	2834	rBV3	5479	5884	0.33%	0.033%
32	20.044	2845	2852	2858	rBV	1270625	1792802	99.97%	9.954%
33	20.274	2889	2891	2894	rBV3	1785	2116	0.12%	0.012%
34	20.309	2895	2897	2900	rVB3	2060	1812	0.10%	0.010%
35	20.338	2900	2902	2905	rBV4	1973	2129	0.12%	0.012%
36	20.567	2940	2941	2944	rVB3	3313	2044	0.11%	0.011%

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Smoothing : OFF

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010423.M
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37	20.608	2944	2948	2951	rBV5	3295	3956	0.22%	0.022%
38	20.638	2951	2953	2954	rBV2	3132	2708	0.15%	0.015%
39	20.732	2967	2969	2972	rVB4	3770	3443	0.19%	0.019%
40	20.961	3006	3008	3012	rVB4	6345	7078	0.39%	0.039%
41	21.026	3017	3019	3020	rBV2	2975	2159	0.12%	0.012%
42	21.243	3043	3056	3069	rBV2	24250	117227	6.54%	0.651%
43	21.484	3095	3097	3098	rBV2	2858	2259	0.13%	0.013%
44	21.554	3107	3109	3113	rBV5	3872	3903	0.22%	0.022%
45	21.925	3169	3172	3173	rBV3	4945	5782	0.32%	0.032%
46	21.972	3173	3180	3188	rVB2	627980	1121208	62.52%	6.225%
47	22.189	3215	3217	3218	rBV2	2985	1978	0.11%	0.011%
48	22.489	3266	3268	3269	rVB2	4071	1853	0.10%	0.010%
49	22.724	3303	3308	3313	rBV7	14769	26930	1.50%	0.150%
50	22.776	3315	3317	3323	rVB7	9656	15731	0.88%	0.087%
51	22.947	3344	3346	3348	rBV3	3353	2606	0.15%	0.014%
52	23.241	3394	3396	3402	rBV7	4633	8631	0.48%	0.048%
53	23.523	3439	3444	3451	rVB7	22164	43854	2.45%	0.243%
54	23.605	3456	3458	3460	rBV3	3380	3962	0.22%	0.022%
55	23.652	3461	3466	3472	rVB6	21055	43939	2.45%	0.244%
56	23.969	3519	3520	3523	rVB3	3644	1832	0.10%	0.010%
57	24.322	3578	3580	3581	rBV2	3946	3169	0.18%	0.018%
58	24.386	3586	3591	3599	rVV3	31039	71434	3.98%	0.397%
59	24.780	3648	3658	3666	rBV5	36173	90547	5.05%	0.503%
60	24.886	3674	3676	3677	rBV2	4495	2169	0.12%	0.012%
61	25.197	3716	3729	3740	rBV2	609720	1793336	100.00%	9.957%
62	25.432	3757	3769	3781	rVB3	379640	1225994	68.36%	6.807%
63	26.061	3875	3876	3877	rBV	4738	2551	0.14%	0.014%
64	26.167	3882	3894	3902	rVV6	37357	135512	7.56%	0.752%
65	26.578	3962	3964	3965	rBV2	4668	2685	0.15%	0.015%
66	26.643	3967	3975	3983	rVB2	44394	135735	7.57%	0.754%
67	27.565	4131	4132	4134	rBV2	5957	3460	0.19%	0.019%
68	27.688	4151	4153	4154	rBV2	4195	2212	0.12%	0.012%
69	27.894	4180	4188	4203	rVB8	35612	151069	8.42%	0.839%
70	28.111	4216	4225	4236	rVB6	41360	153771	8.57%	0.854%
71	29.880	4518	4526	4527	rBV7	25793	47587	2.65%	0.264%
72	30.074	4551	4559	4560	rBV5	23005	44115	2.46%	0.245%
73	30.420	4616	4618	4619	rBV2	3815	2456	0.14%	0.014%
74	31.643	4824	4826	4827	rVB2	4021	1858	0.10%	0.010%
75	32.042	4890	4894	4895	rBV3	8079	12038	0.67%	0.067%

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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

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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010423.M
Title : SVOA CALIBRATION

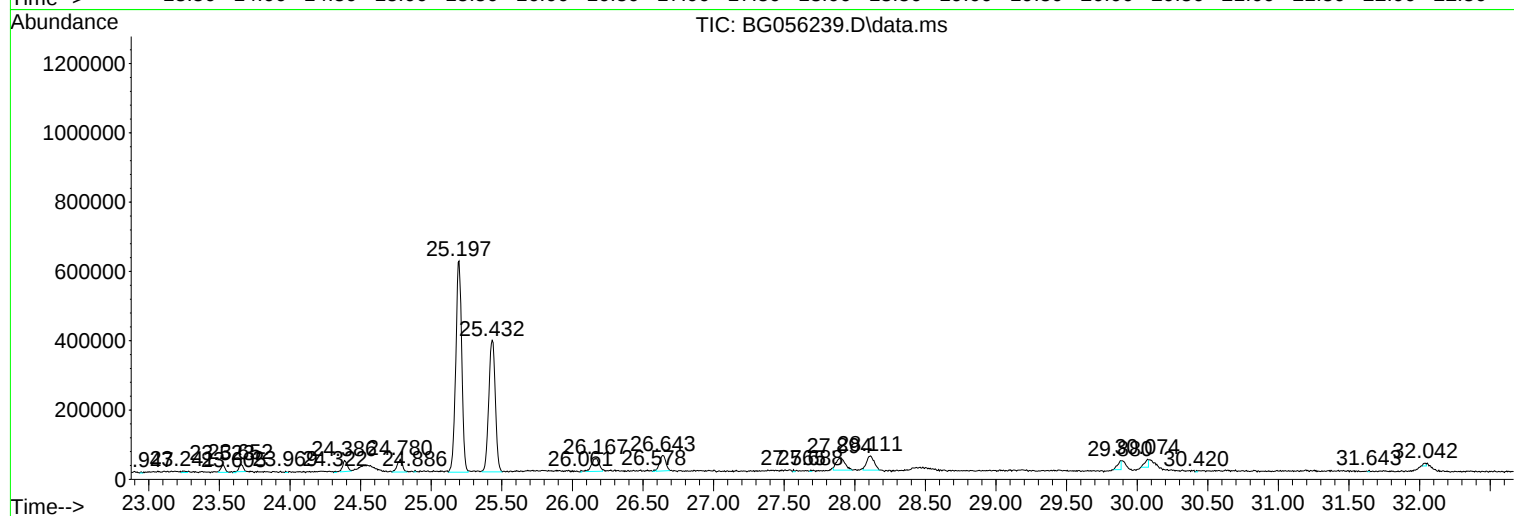
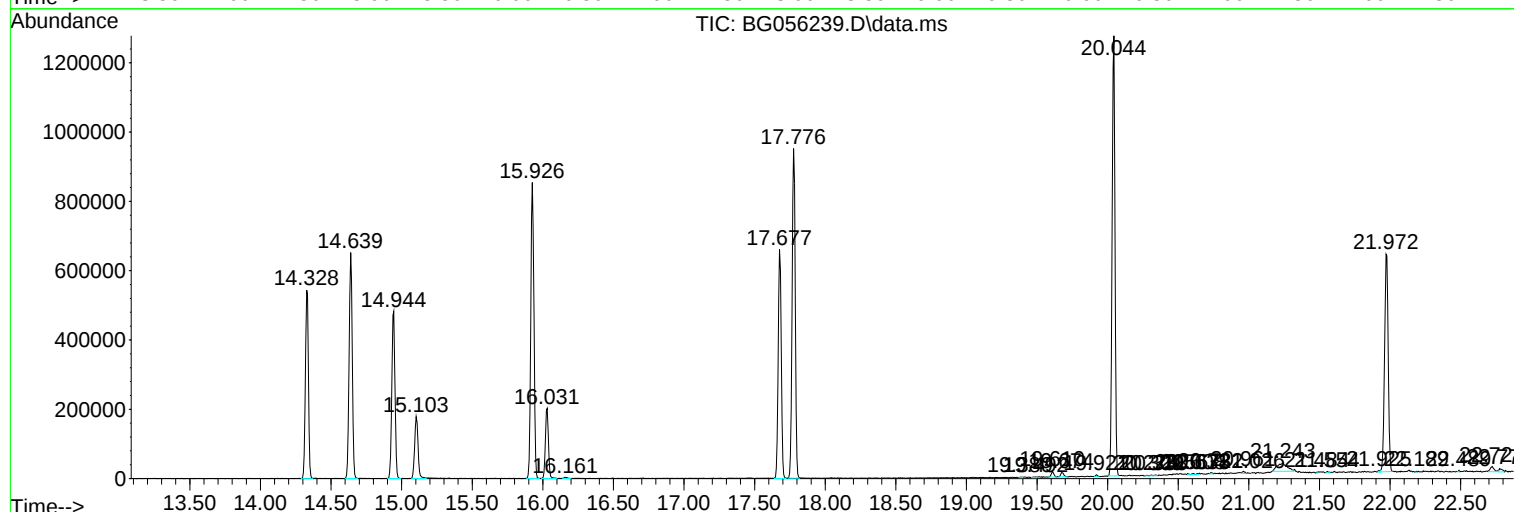
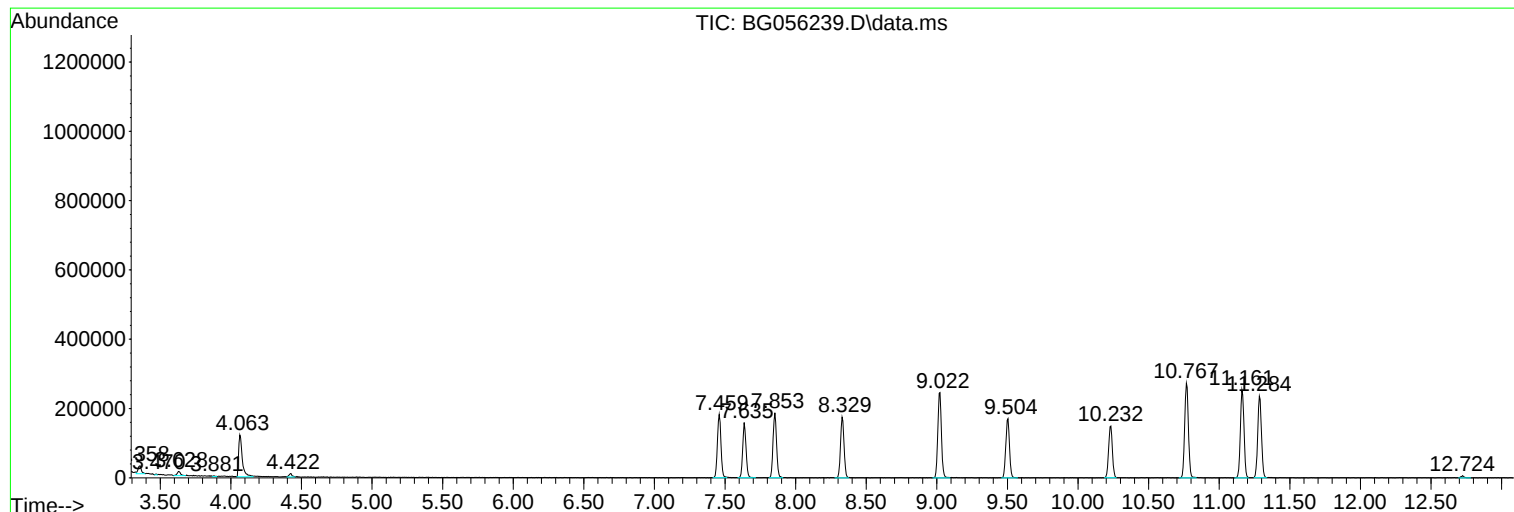
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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010423.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011023\
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Operator : CG/JU
Sample : PB150093BL
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Instrument :
BNA_G
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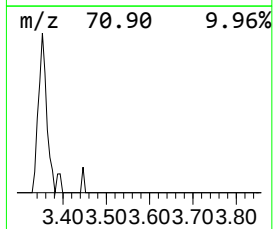
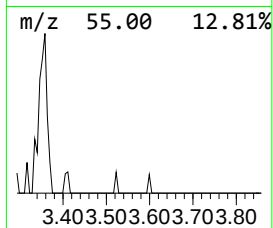
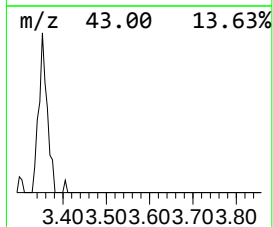
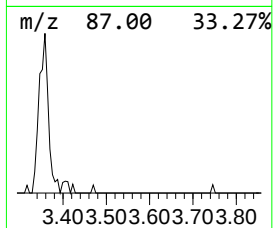
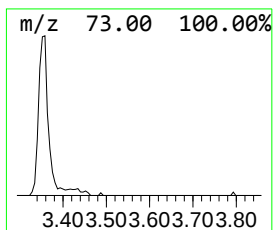
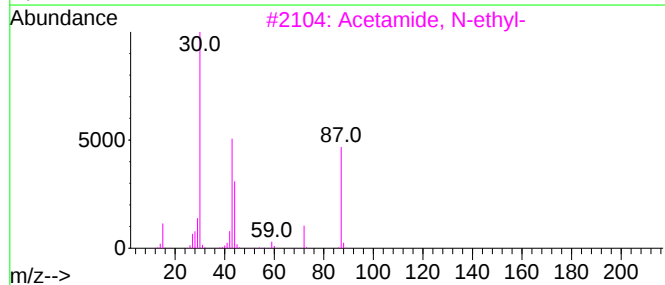
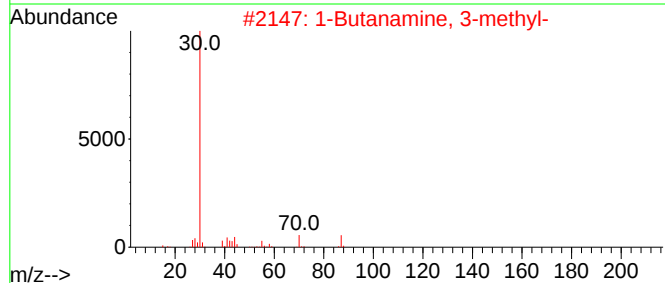
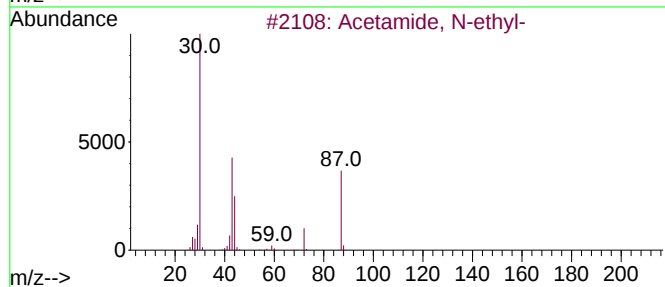
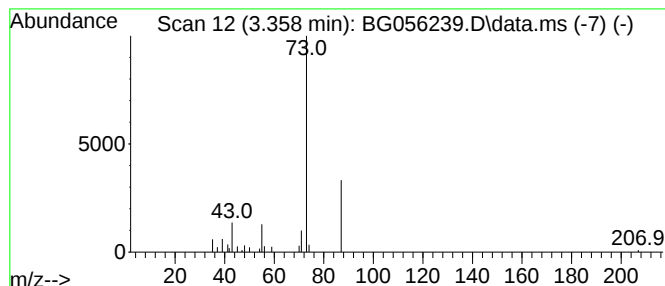
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010423.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.358	2.41 ng/ul	36861	1,4-Dichlorobenzene-d4	8.329

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-ethyl-		87	C4H9NO		000625-50-3	5
2	1-Butanamine, 3-methyl-		87	C5H13N		000107-85-7	5
3	Acetamide, N-ethyl-		87	C4H9NO		000625-50-3	4
4	N-Ethylformamide		73	C3H7NO		000627-45-2	4
5	1-Pentanamine		87	C5H13N		000110-58-7	4



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Misc :
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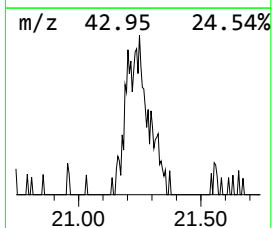
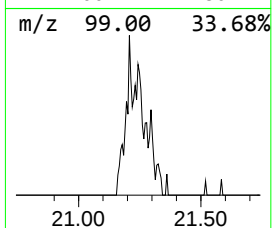
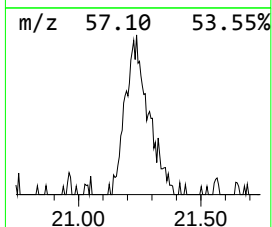
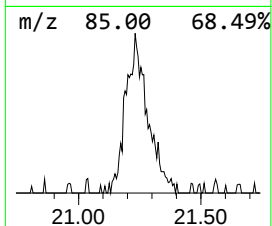
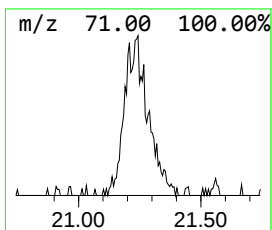
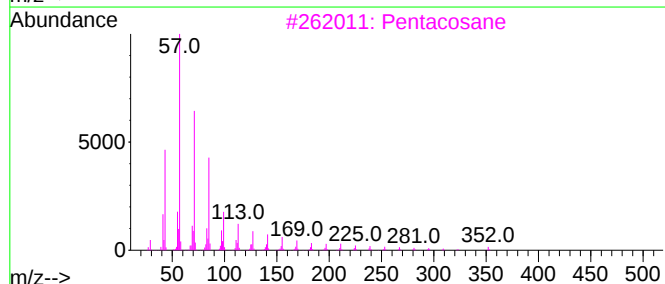
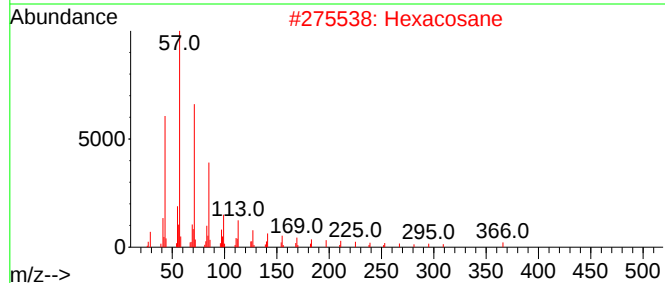
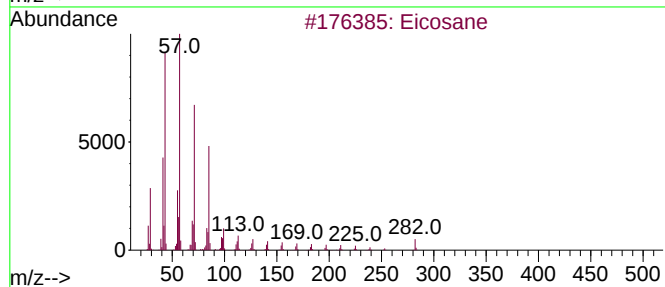
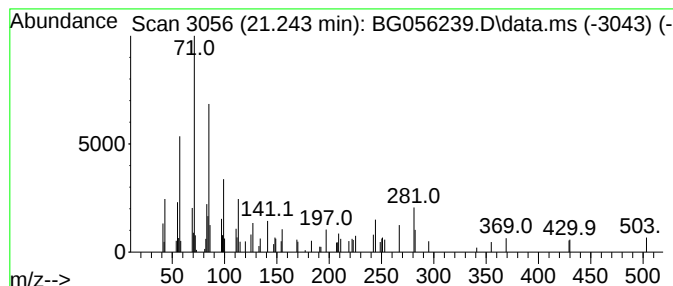
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010423.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.243	2.09 ng/ul	117227	Chrysene-d12		21.972	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	70
2	Hexacosane		366	C26H54	000630-01-3	68
3	Pentacosane		352	C25H52	000629-99-2	68
4	Docosane		310	C22H46	000629-97-0	64
5	Heptacosane		380	C27H56	000593-49-7	64



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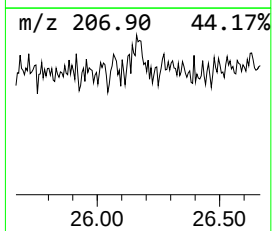
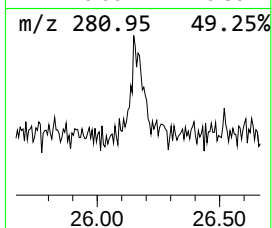
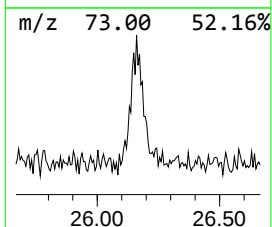
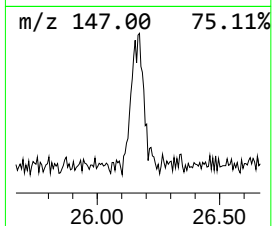
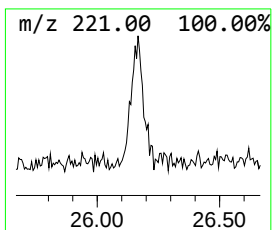
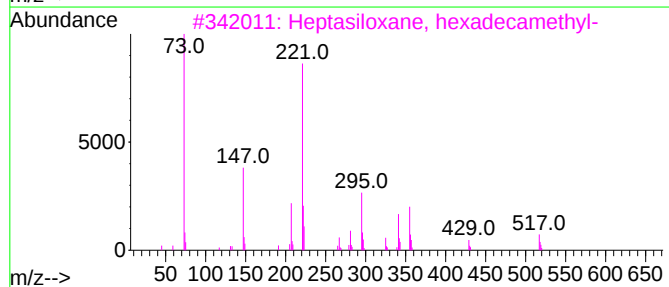
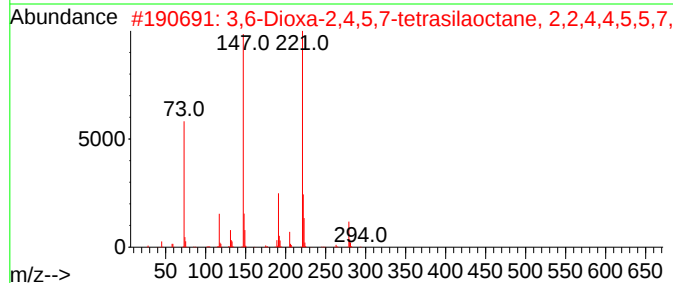
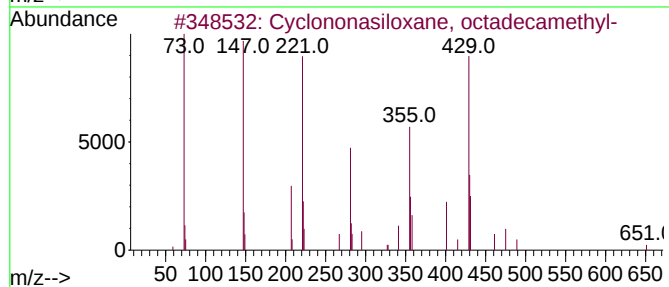
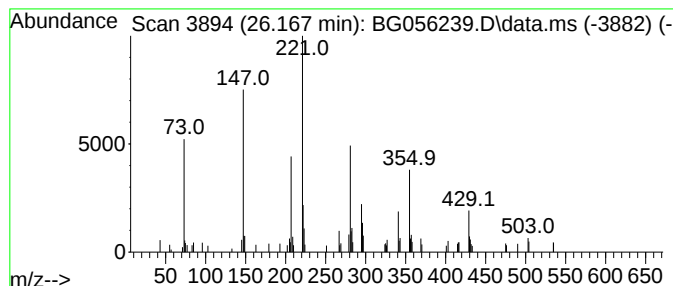
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010423.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Cyclononasiloxane, octadeca... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.167	2.21 ng/ul	135512	Perylene-d12	25.438

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
2			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	35
4			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	32
5			Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	14



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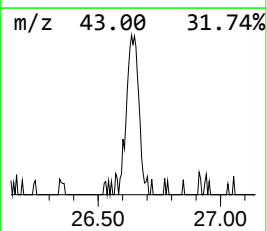
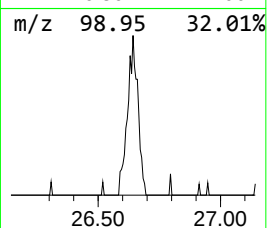
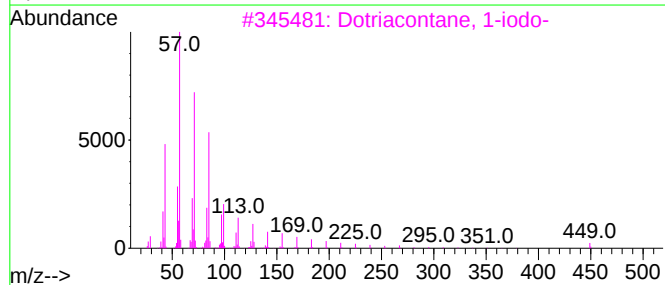
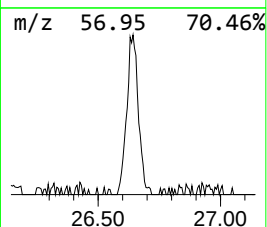
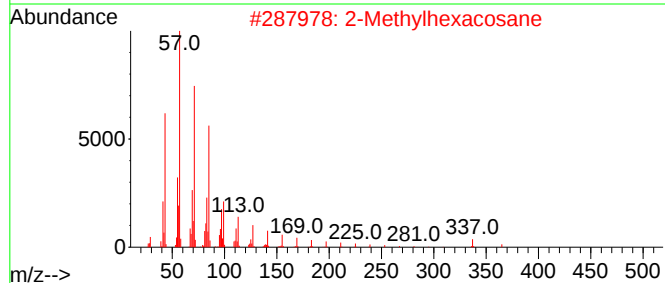
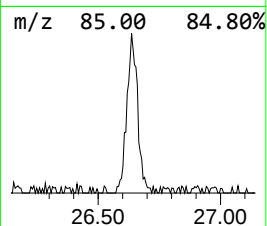
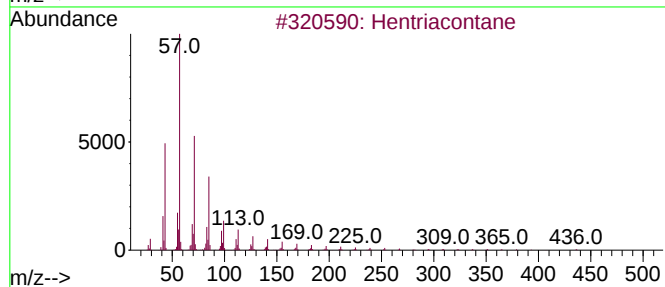
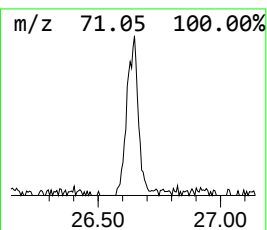
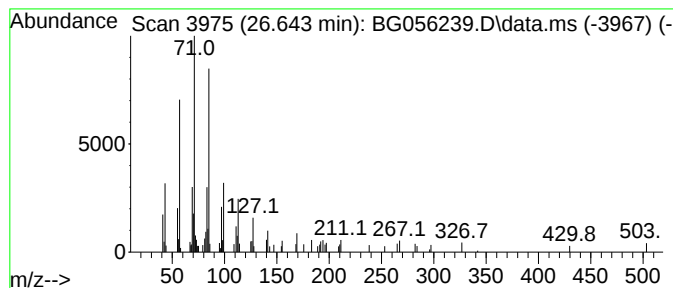
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.643	2.21 ng/ul	135735	Perylene-d12	25.438

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	90
2			2-Methylhexacosane	380	C27H56	001561-02-0	87
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87
4			Octacosane	394	C28H58	000630-02-4	87
5			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011023\
Data File : BG056239.D
Acq On : 10 Jan 2023 11:38
Operator : CG/JU
Sample : PB150093BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SBLK093

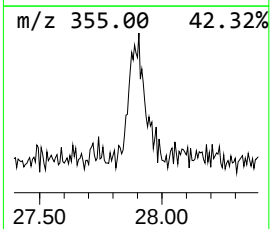
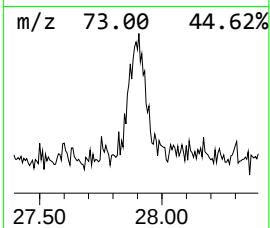
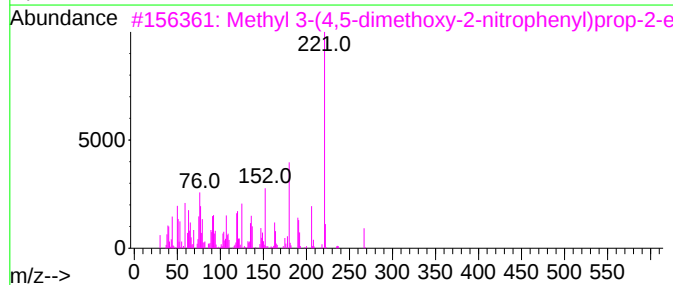
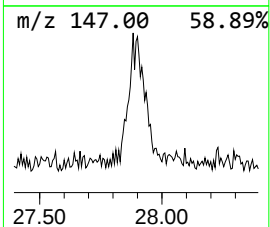
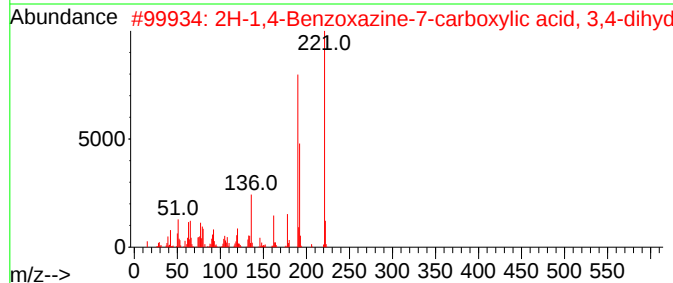
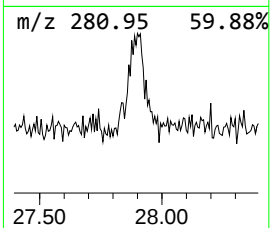
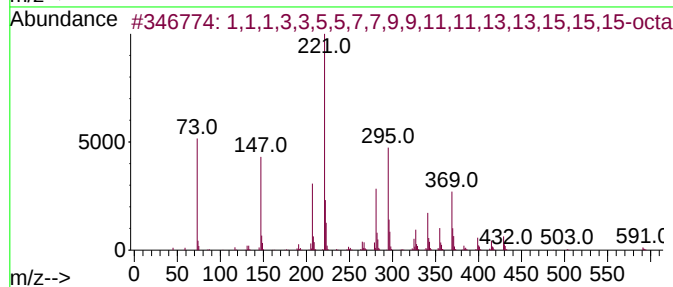
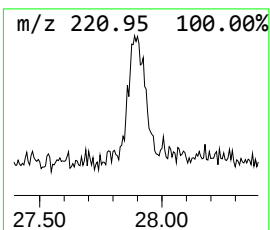
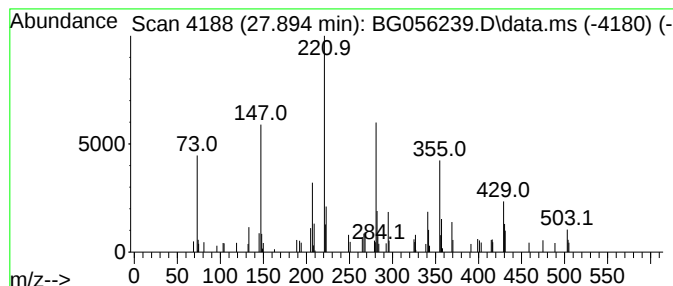
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.894	2.46 ng/ul	151069	Perylene-d12	25.438

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	38		
2	2H-1,4-Benzoxazine-7-carboxylic ...	221	C11H11NO4	201294-27-1	25		
3	Methyl 3-(4,5-dimethoxy-2-nitrop...	267	C12H13NO6	118509-96-9	22		
4	3-Amino-4,6-dimethylthieno[2,3-b...	221	C10H11N3OS	067795-42-0	22		
5	3-Benzylidene-2-indolinone	221	C15H11NO	003359-49-7	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011023\
Data File : BG056239.D
Acq On : 10 Jan 2023 11:38
Operator : CG/JU
Sample : PB150093BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SBLK093

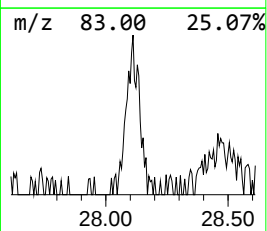
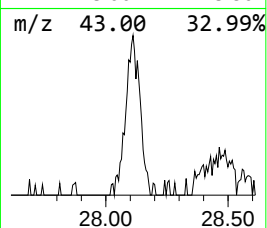
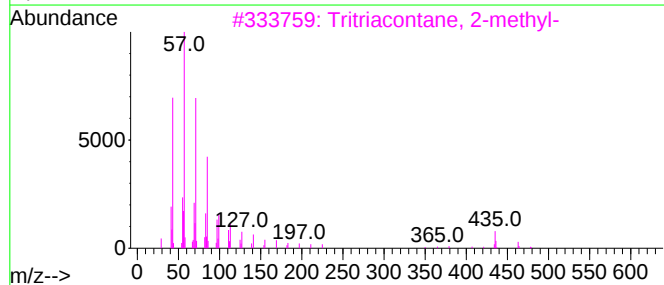
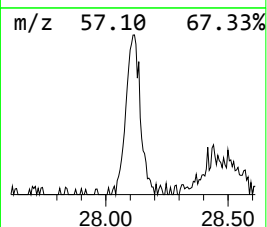
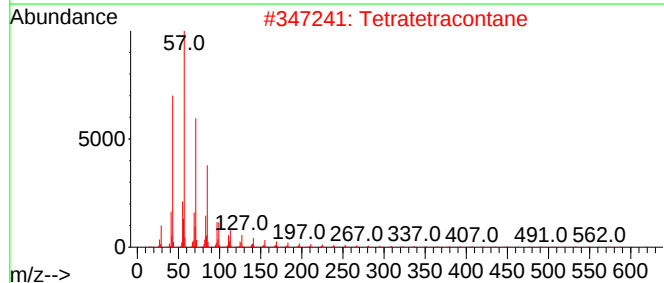
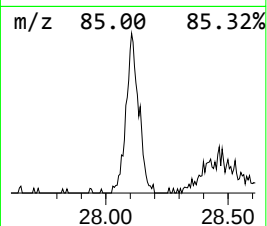
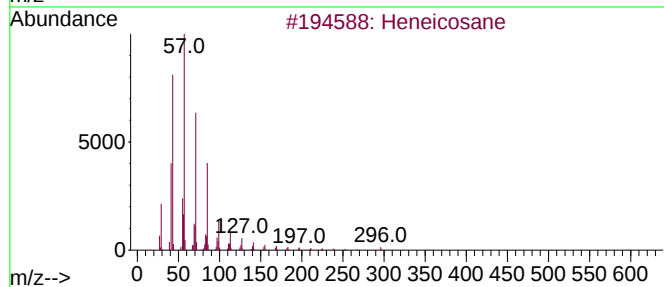
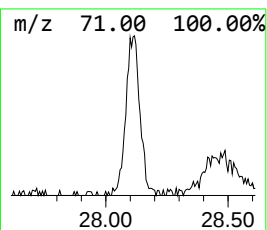
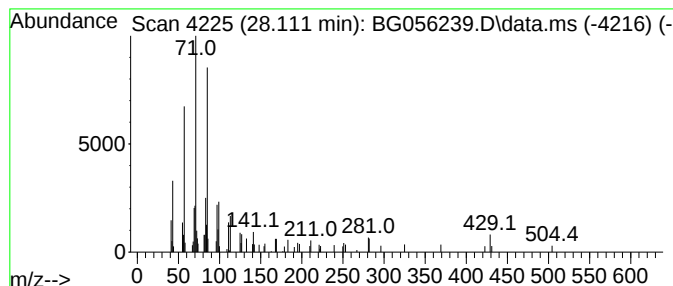
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010423.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.111	2.51 ng/ul	153771	Perylene-d12	25.438

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Tetratetracontane	619	C44H90	007098-22-8	87
3			Trtriacontane, 2-methyl-	479	C34H70	066214-27-5	86
4			Tetratriacontane, 2-methyl-	493	C35H72	014167-65-8	86
5			Hexatriacontane	507	C36H74	000630-06-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011023\
Data File : BG056239.D
Acq On : 10 Jan 2023 11:38
Operator : CG/JU
Sample : PB150093BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SBLK093

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG010423.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
unknown-01	3.358	2.4	ng/u1	36861	1	8.329	305358	20.0
(DEL) Alkane: S...	21.243	2.1	ng/u1	117227	5	21.972	1121210	20.0
Cyclononasiloxa...	26.167	2.2	ng/u1	135512	6	25.438	1225990	20.0
(DEL) Alkane: S...	26.643	2.2	ng/u1	135735	6	25.438	1225990	20.0
unknown-02	27.894	2.5	ng/u1	151069	6	25.438	1225990	20.0
(DEL) Alkane: S...	28.111	2.5	ng/u1	153771	6	25.438	1225990	20.0