

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
 Data File : BG059672.D
 Acq On : 6 Nov 2023 3:12
 Operator : MA/JU
 Sample : 04948-03
 Misc :
 ALS Vial : 64 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0AH5

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-BG110323.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG059672.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.568	29	30	33	rBV3	6988	6341	0.71%	0.079%
2	3.615	33	38	41	rVV4	8995	17225	1.92%	0.216%
3	4.138	126	127	130	rVB	6082	4033	0.45%	0.050%
4	4.308	153	156	158	rBV3	9595	10281	1.15%	0.129%
5	4.414	172	174	176	rBV3	3991	3936	0.44%	0.049%
6	4.613	207	208	210	rBV	3735	3577	0.40%	0.045%
7	4.631	210	211	213	rVB	6562	3397	0.38%	0.043%
8	4.790	236	238	239	rBV	6686	4298	0.48%	0.054%
9	5.107	288	292	293	rBV	5372	4284	0.48%	0.054%
10	5.307	323	326	329	rVB	4191	4708	0.53%	0.059%
11	5.354	329	334	336	rBV2	8502	11201	1.25%	0.140%
12	5.465	349	353	355	rBV	4055	6077	0.68%	0.076%
13	5.677	387	389	391	rBV	6315	3993	0.45%	0.050%
14	5.700	391	393	395	rVB	7131	4844	0.54%	0.061%
15	5.718	395	396	399	rBV	5033	6054	0.68%	0.076%
16	5.912	426	429	435	rBV5	14259	30812	3.44%	0.386%
17	6.159	470	471	474	rBV	9560	5036	0.56%	0.063%
18	6.494	526	528	529	rBV	5807	4152	0.46%	0.052%
19	6.552	535	538	539	rBV	7717	7336	0.82%	0.092%
20	6.711	562	565	566	rBV	6170	5838	0.65%	0.073%
21	7.205	647	649	653	rBV	3147	4196	0.47%	0.053%
22	7.281	660	662	664	rBV	5958	4902	0.55%	0.061%
23	7.393	679	681	683	rVB2	7326	4187	0.47%	0.052%
24	7.457	687	692	700	rBV2	88404	164761	18.38%	2.062%
25	7.663	717	727	734	rBV2	81445	169075	18.86%	2.116%
26	7.810	751	752	755	rBV	5545	3388	0.38%	0.042%
27	7.863	755	761	770	rVV2	123032	231500	25.83%	2.898%
28	7.962	773	778	781	rBV3	19006	27619	3.08%	0.346%
29	8.062	793	795	797	rBV3	5844	3888	0.43%	0.049%
30	8.350	838	844	850	rVB2	144207	240682	26.85%	3.013%
31	8.397	850	852	855	rVB	8735	7265	0.81%	0.091%
32	8.444	855	860	863	rBV3	11173	17668	1.97%	0.221%
33	8.703	901	904	906	rBV	5368	7160	0.80%	0.090%
34	9.032	955	960	968	rVB2	66793	123160	13.74%	1.542%
35	9.196	982	988	999	rVB4	54909	121610	13.57%	1.522%
36	9.267	999	1000	1003	rBV3	7607	7961	0.89%	0.100%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
 Data File : BG059672.D
 Acq On : 6 Nov 2023 3:12
 Operator : MA/JU
 Sample : 04948-03
 Misc :
 ALS Vial : 64 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0AH5

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-BG110323.MA.M
 Title : SVOA CALIBRATION

37	9.326	1008	1010	1011	rBV	8035	4838	0.54%	0.061%
38	9.543	1042	1047	1054	rVB2	131657	233213	26.02%	2.919%
39	9.690	1071	1072	1074	rBV2	6165	5424	0.61%	0.068%
40	9.872	1101	1103	1106	rVB2	7504	7997	0.89%	0.100%
41	9.913	1106	1110	1113	rBV2	5584	9803	1.09%	0.123%
42	10.101	1141	1142	1145	rBV2	4300	3847	0.43%	0.048%
43	10.195	1156	1158	1160	rBV	6099	4907	0.55%	0.061%
44	10.266	1165	1170	1178	rVB4	123925	213053	23.77%	2.667%
45	10.430	1196	1198	1199	rBV	8703	5879	0.66%	0.074%
46	10.695	1242	1243	1246	rBV	5493	4804	0.54%	0.060%
47	10.747	1251	1252	1253	rVV	8387	3634	0.41%	0.045%
48	10.794	1253	1260	1269	rVB3	164693	322268	35.95%	4.034%
49	10.859	1269	1271	1273	rBV	6042	7647	0.85%	0.096%
50	11.194	1322	1328	1335	rBV	186252	351269	39.19%	4.397%
51	11.294	1343	1345	1347	rBV	4679	4796	0.54%	0.060%
52	11.341	1347	1353	1361	rVB3	99037	201684	22.50%	2.524%
53	11.975	1459	1461	1462	rBV	6090	4688	0.52%	0.059%
54	12.075	1476	1478	1480	rBV2	6996	6896	0.77%	0.086%
55	12.246	1505	1507	1510	rVB2	7558	7352	0.82%	0.092%
56	12.669	1576	1579	1583	rBV2	8322	10992	1.23%	0.138%
57	13.215	1669	1672	1673	rBV2	3776	3600	0.40%	0.045%
58	13.274	1680	1682	1684	rBV2	6393	5924	0.66%	0.074%
59	13.374	1696	1699	1703	rBV2	3233	5941	0.66%	0.074%
60	13.421	1706	1707	1710	rBV2	6373	4906	0.55%	0.061%
61	13.609	1735	1739	1742	rBV2	6317	10080	1.12%	0.126%
62	13.809	1763	1773	1778	rBV4	51195	87557	9.77%	1.096%
63	14.120	1825	1826	1827	rBV4	8468	4370	0.49%	0.055%
64	14.373	1863	1869	1874	rVB	270933	399837	44.61%	5.005%
65	14.467	1882	1885	1888	rVB	4053	4718	0.53%	0.059%
66	14.561	1898	1901	1903	rBV	4201	3330	0.37%	0.042%
67	14.578	1903	1904	1909	rBV	2407	3888	0.43%	0.049%
68	14.678	1915	1921	1928	rVB2	277832	440154	49.11%	5.509%
69	14.913	1958	1961	1963	rVB2	3369	3787	0.42%	0.047%
70	14.937	1963	1965	1966	rBV2	6716	4777	0.53%	0.060%
71	14.978	1966	1972	1977	rVV	258603	387151	43.19%	4.846%
72	15.078	1986	1989	1993	rBV	4656	4776	0.53%	0.060%
73	15.148	1995	2001	2009	rBV2	141589	216905	24.20%	2.715%
74	15.324	2028	2031	2036	rVB3	10431	16706	1.86%	0.209%
75	15.377	2038	2040	2045	rVV4	8546	10479	1.17%	0.131%
76	15.413	2045	2046	2050	rVB2	3765	4526	0.50%	0.057%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
 Data File : BG059672.D
 Acq On : 6 Nov 2023 3:12
 Operator : MA/JU
 Sample : 04948-03
 Misc :
 ALS Vial : 64 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0AH5

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-BG110323.MA.M
 Title : SVOA CALIBRATION

77	15.577	2073	2074	2076	rBV2	3818	3803	0.42%	0.048%
78	15.771	2106	2107	2110	rBV2	3875	3323	0.37%	0.042%
79	15.847	2117	2120	2121	rBV	4154	4253	0.47%	0.053%
80	15.965	2134	2140	2149	rBV2	354314	537598	59.98%	6.729%
81	16.065	2152	2157	2163	rVB2	114285	159529	17.80%	1.997%
82	16.429	2217	2219	2222	rBV3	3911	4033	0.45%	0.050%
83	16.829	2285	2287	2289	rBV3	5274	4833	0.54%	0.060%
84	16.858	2290	2292	2295	rBV	4893	4392	0.49%	0.055%
85	16.940	2302	2306	2311	rVB	5983	12217	1.36%	0.153%
86	17.011	2316	2318	2321	rBV	7008	5214	0.58%	0.065%
87	17.163	2339	2344	2346	rBV	4966	8308	0.93%	0.104%
88	17.234	2353	2356	2363	rVB4	18595	29994	3.35%	0.375%
89	17.504	2400	2402	2404	rBV	4051	3756	0.42%	0.047%
90	17.727	2432	2440	2445	rBV	331400	506064	56.46%	6.334%
91	17.827	2451	2457	2463	rBV2	348096	533435	59.51%	6.677%
92	18.086	2499	2501	2505	rBV3	7603	9700	1.08%	0.121%
93	18.180	2514	2517	2518	rBV3	3880	3938	0.44%	0.049%
94	18.544	2574	2579	2590	rBV2	98814	147311	16.43%	1.844%
95	19.326	2710	2712	2715	rBV4	6292	8251	0.92%	0.103%
96	19.378	2719	2721	2726	rVB5	13387	18364	2.05%	0.230%
97	19.490	2736	2740	2744	rBV6	33775	56360	6.29%	0.705%
98	19.802	2790	2793	2800	rVB5	54096	74359	8.30%	0.931%
99	20.101	2839	2844	2852	rVB	586088	896334	100.00%	11.219%
100	22.058	3173	3177	3188	rVB	352856	629005	70.18%	7.873%

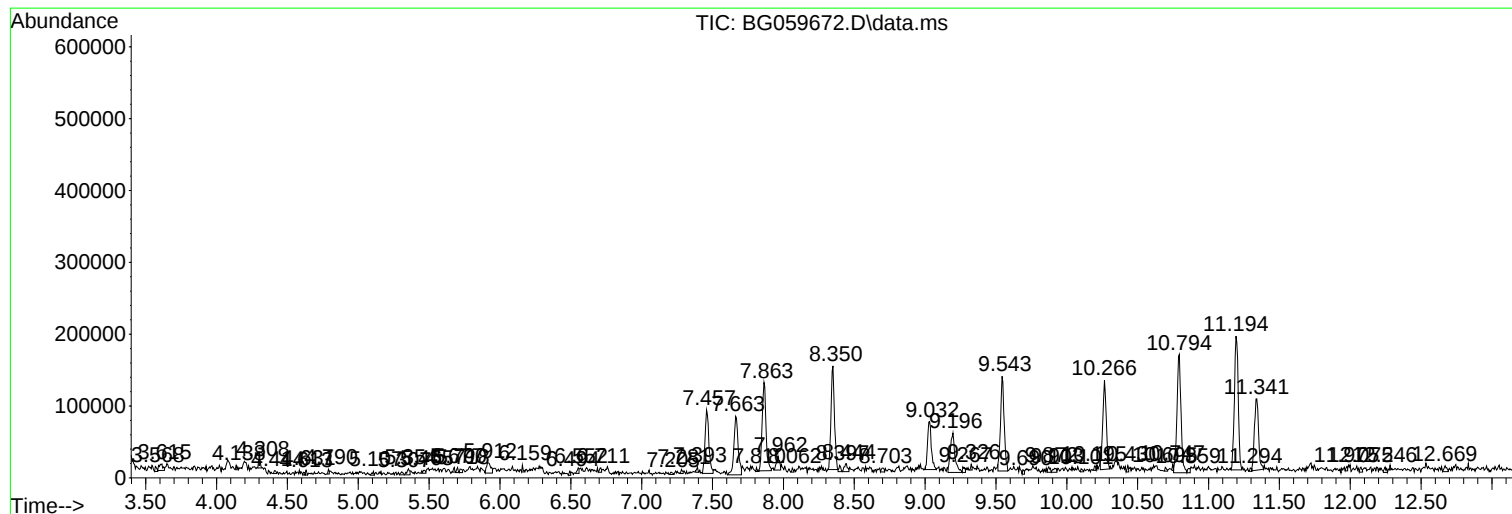
Sum of corrected areas: 7989222

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
Data File : BG059672.D
Acq On : 6 Nov 2023 3:12
Operator : MA/JU
Sample : 04948-03
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COAH5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
Data File : BG059672.D
Acq On : 6 Nov 2023 3:12
Operator : MA/JU
Sample : 04948-03
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AH5

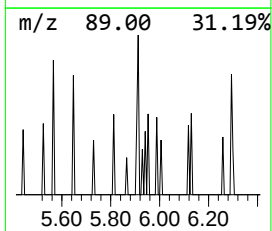
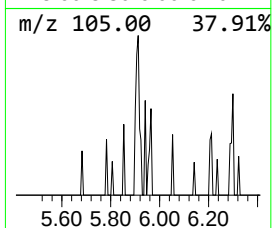
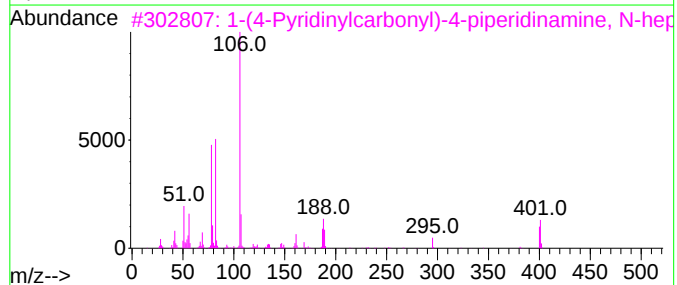
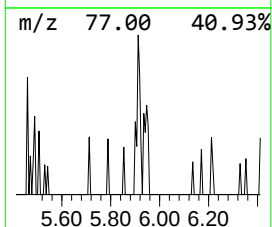
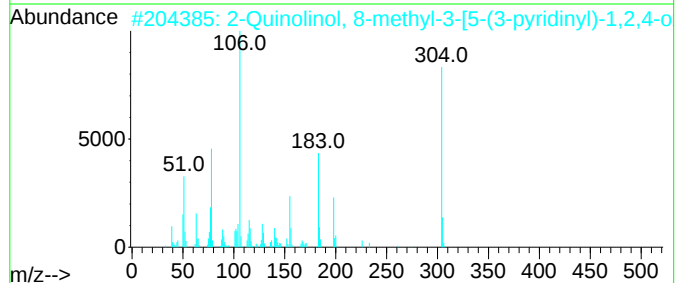
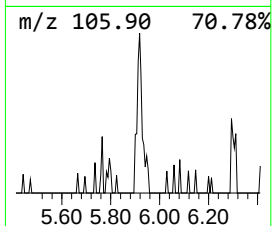
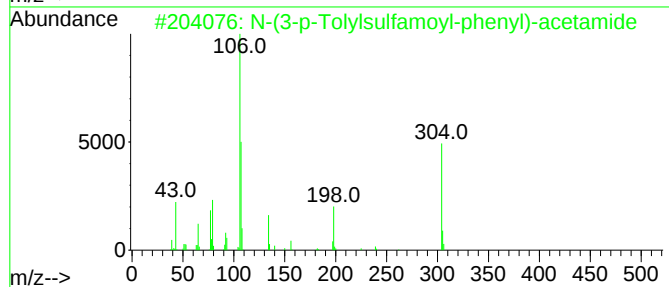
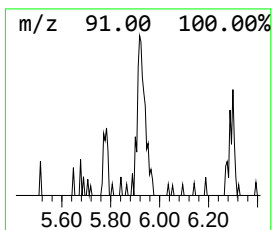
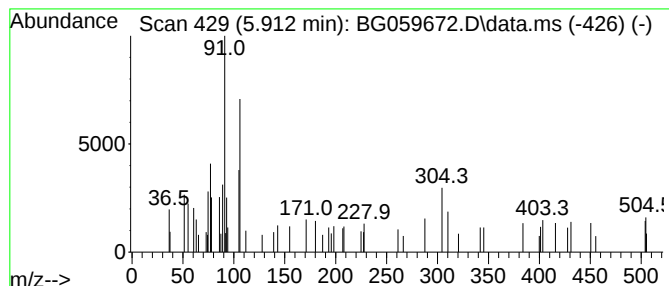
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.912	2.56 ng/ul	30812	1,4-Dichlorobenzene-d4	8.350

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(3-p-Tolylsulfamoyl-phenyl)-ac...	304	C15H16N2O3S	1000317-85-8	27
2			2-Quinolinol, 8-methyl-3-[5-(3-p...	304	C17H12N4O2	1000319-71-6	27
3			1-(4-Pyridinylcarbonyl)-4-piperi...	401	C15H14F7N3O2	1010469-18-0	22
4			3,3,4-Tricyano-4a-methyl-2-pheny...	345	C20H19N5O	1000409-46-4	9
5			propanoic acid, 3-hydroxy-2-(hyd...	345	C14H23N3O5S	1000398-27-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
Data File : BG059672.D
Acq On : 6 Nov 2023 3:12
Operator : MA/JU
Sample : 04948-03
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AH5

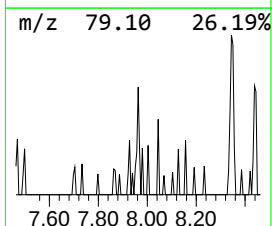
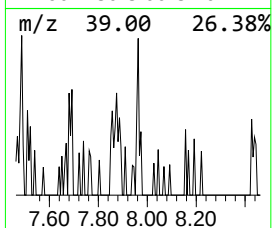
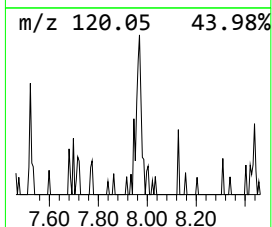
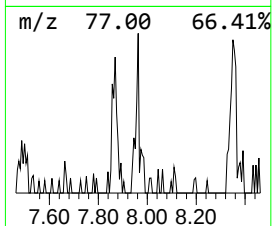
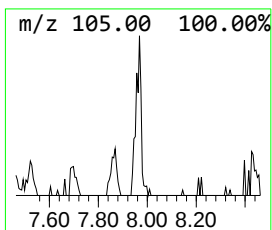
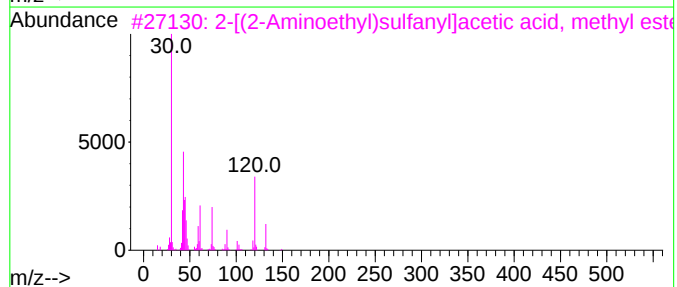
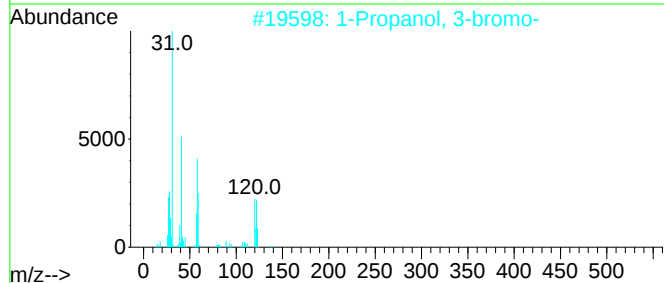
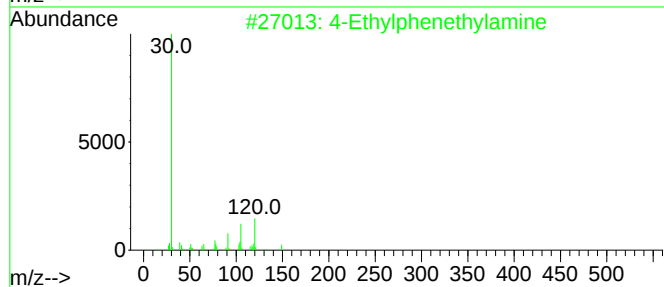
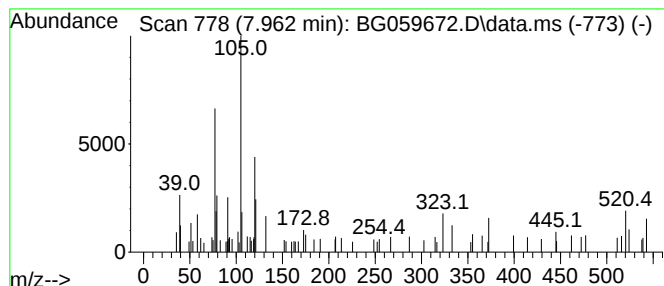
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.962	2.30 ng/ul	27619	1,4-Dichlorobenzene-d4	8.350

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Ethylphenethylamine	149	C10H15N	064353-29-3	4
2		1-Propanol, 3-bromo-	138	C3H7BrO	000627-18-9	1
3		2-[(2-Aminoethyl)sulfanyl]acetic...	149	C5H11NO2S	366446-58-4	1
4		Benzeneethanamine, 2-chloro-	155	C8H10ClN	013078-80-3	1
5		2,5-Dichloropentylamine	155	C5H11Cl2N	108766-06-9	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
Data File : BG059672.D
Acq On : 6 Nov 2023 3:12
Operator : MA/JU
Sample : 04948-03
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AH5

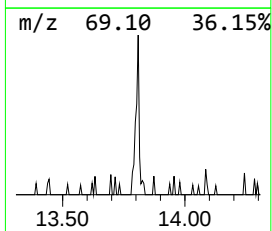
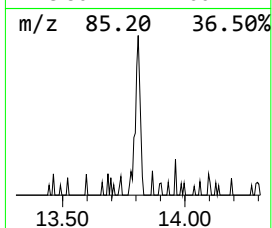
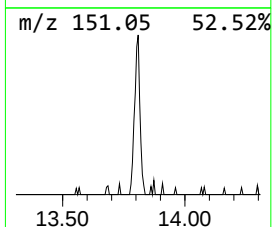
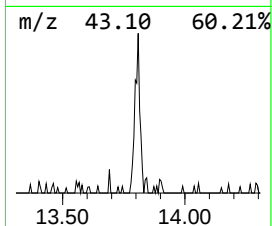
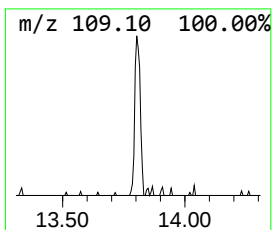
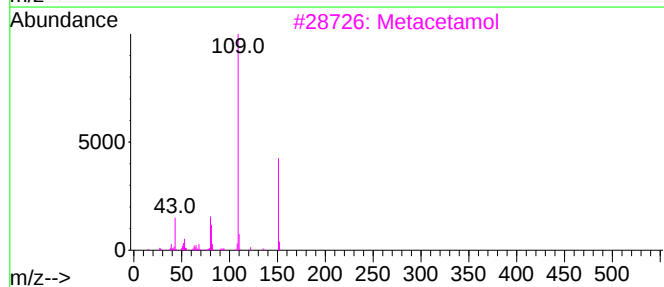
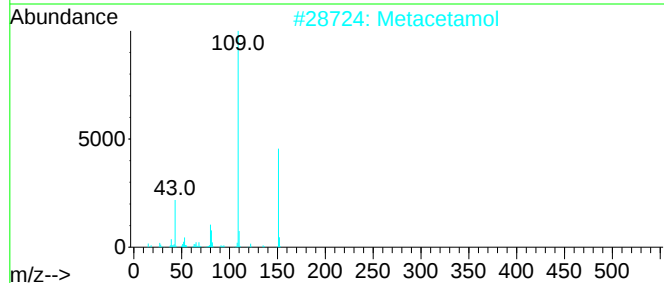
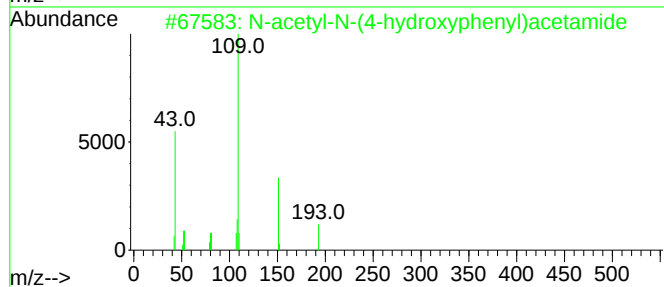
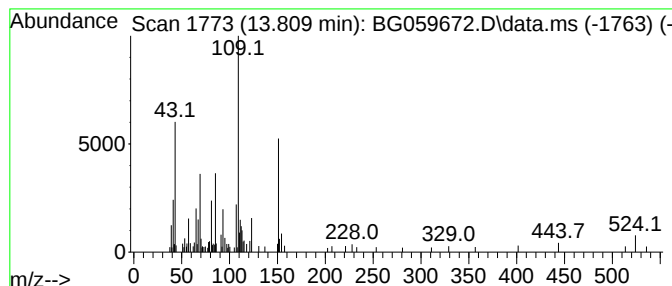
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 N-acetyl-N-(4-hydroxyphenyl)... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.809	4.52 ng/ul	87557	Acenaphthene-d10	14.978

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-acetyl-N-(4-hydroxyphenyl)acet...	193	C10H11NO3	1000389-51-9	50
2			Metacetamol	151	C8H9NO2	000621-42-1	49
3			Metacetamol	151	C8H9NO2	000621-42-1	49
4			Metacetamol	151	C8H9NO2	000621-42-1	49
5			m-Isopropoxyaniline	151	C9H13NO	041406-00-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
Data File : BG059672.D
Acq On : 6 Nov 2023 3:12
Operator : MA/JU
Sample : 04948-03
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AH5

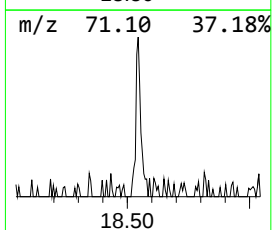
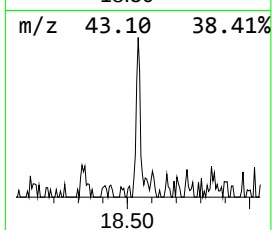
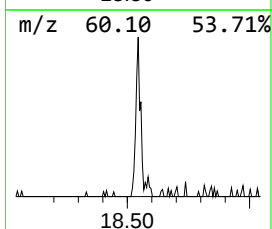
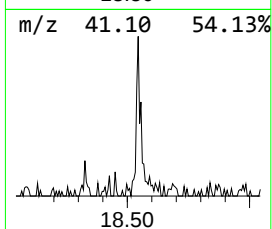
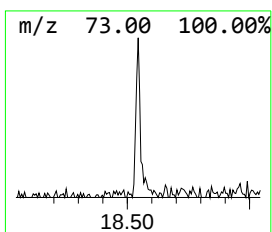
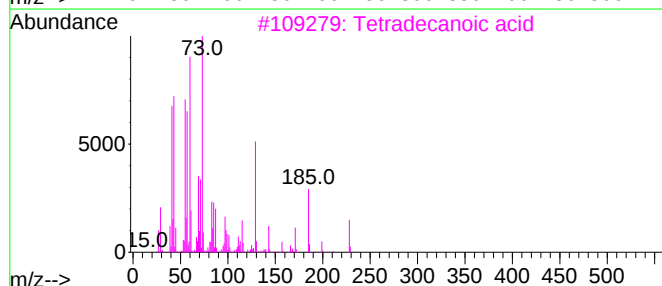
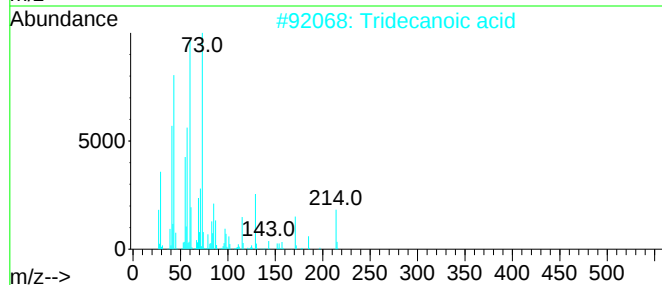
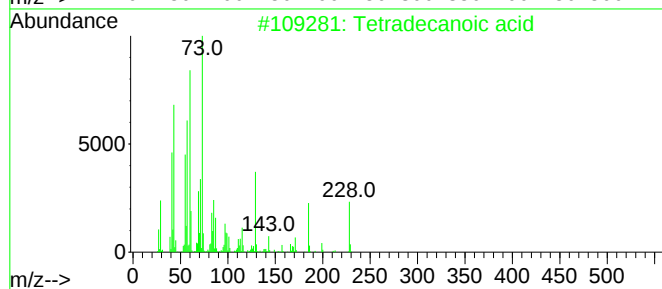
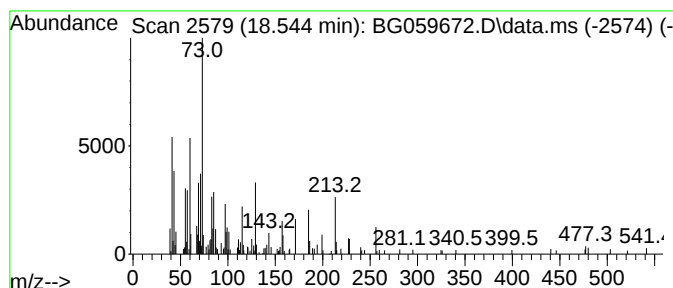
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 Tetradecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.544	5.82 ng/ul	147311	Phenanthrene-d10	17.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
2			Tridecanoic acid	214	C13H26O2	000638-53-9	55
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
Data File : BG059672.D
Acq On : 6 Nov 2023 3:12
Operator : MA/JU
Sample : 04948-03
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AH5

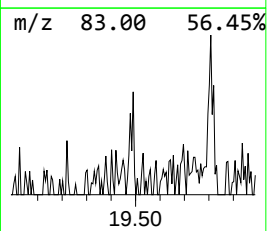
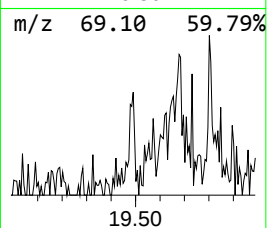
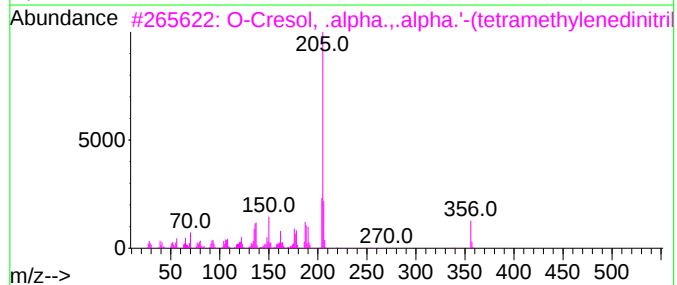
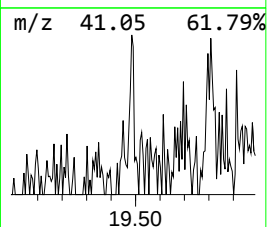
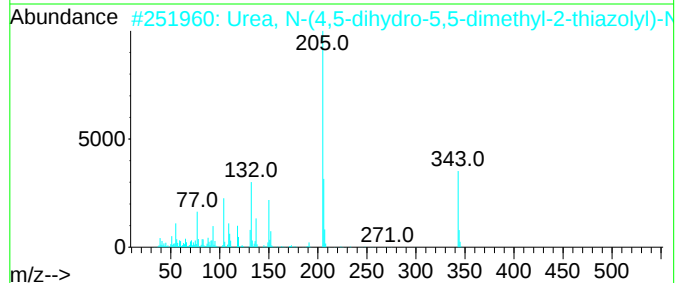
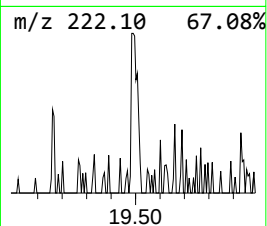
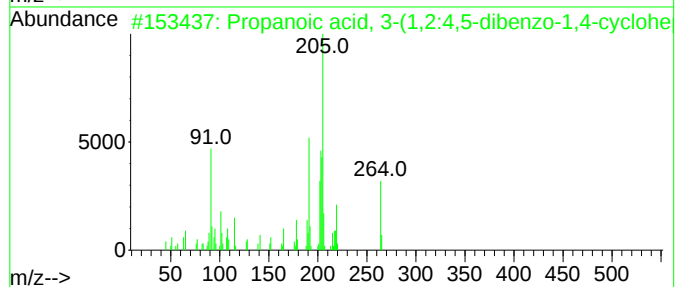
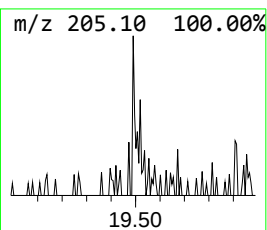
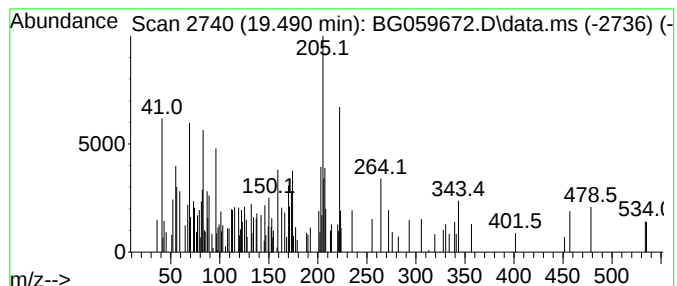
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-03 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.490	2.23 ng/ul	56360	Phenanthrene-d10	17.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 3-(1,2:4,5-diben...	264	C18H16O2	040443-03-6	30
2			Urea, N-(4,5-dihydro-5,5-dimethy...	343	C18H18FN3OS	1000351-05-3	27
3			O-Cresol, .alpha.,.alpha.'-(tetr...	356	C20H24N2O4	104978-24-7	18
4			5-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-92-1	18
5			6-(4-Methoxy-phenyl)-2H-[1,3]thi...	205	C11H11NOS	1000287-40-3	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
Data File : BG059672.D
Acq On : 6 Nov 2023 3:12
Operator : MA/JU
Sample : 04948-03
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AH5

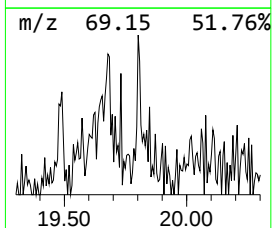
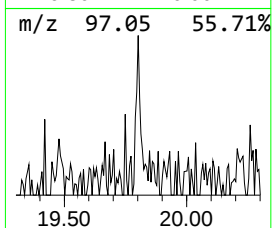
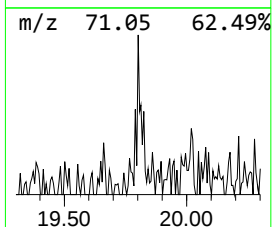
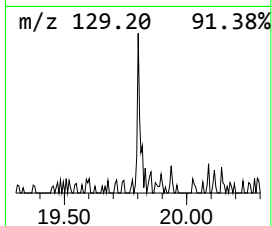
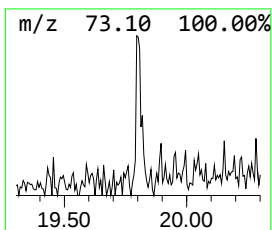
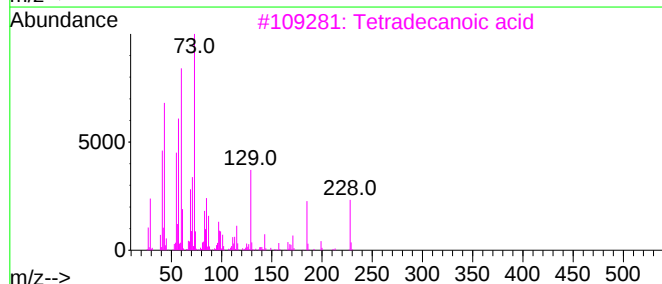
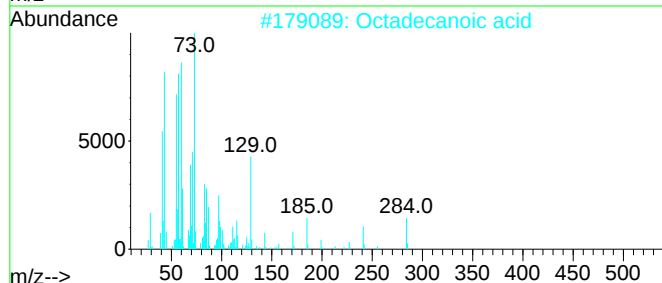
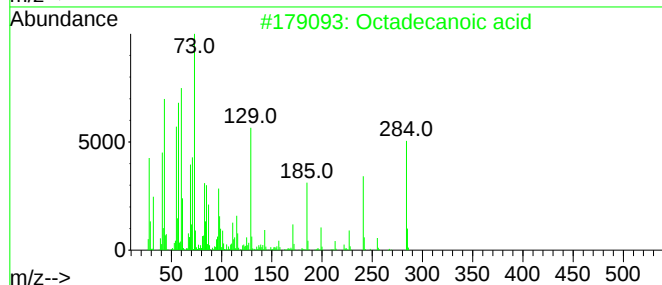
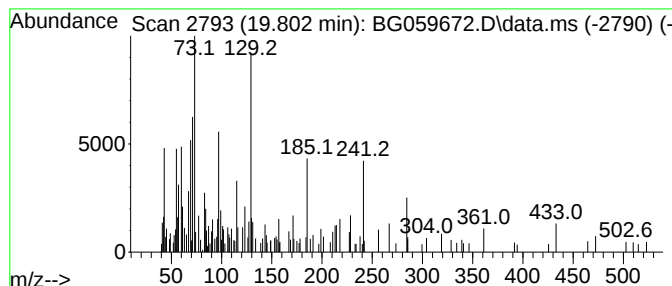
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.802	2.94 ng/ul	74359	Phenanthrene-d10	17.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	90
2			Octadecanoic acid	284	C18H36O2	000057-11-4	70
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4			Adipic acid, butyl trans-2-methy...	298	C17H30O4	1000324-74-6	43
5			Adipic acid, butyl cycloheptyl e...	298	C17H30O4	1000324-71-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110423\
Data File : BG059672.D
Acq On : 6 Nov 2023 3:12
Operator : MA/JU
Sample : 04948-03
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AH5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG110323.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
unknown-01	5.912	2.6	ng/ul	30812	1	8.350	240682	20.0
unknown-02	7.962	2.3	ng/ul	27619	1	8.350	240682	20.0
N-acetyl-N-(4-h...	13.809	4.5	ng/ul	87557	3	14.978	387151	20.0
Tetradecanoic acid	18.544	5.8	ng/ul	147311	4	17.727	506064	20.0
unknown-03	19.490	2.2	ng/ul	56360	4	17.727	506064	20.0
Octadecanoic acid	19.802	2.9	ng/ul	74359	4	17.727	506064	20.0