

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092023\
 Data File : BG059159.D
 Acq On : 22 Sep 2023 11:07
 Operator : MA/JU
 Sample : 04386-14
 Misc :
 ALS Vial : 61 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0AM9

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-BG091923.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG059159.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.606	33	37	42	rVB2	11486	17993	1.97%	0.175%
2	3.888	83	85	87	rBV3	3650	3025	0.33%	0.029%
3	4.035	106	110	119	rBV	166286	268466	29.41%	2.615%
4	4.205	137	139	142	rBV3	3126	3244	0.36%	0.032%
5	4.258	145	148	152	rVB3	4692	5952	0.65%	0.058%
6	4.452	180	181	184	rBV2	1916	1611	0.18%	0.016%
7	4.516	189	192	193	rVB3	2703	2365	0.26%	0.023%
8	4.751	229	232	238	rVB5	3319	5804	0.64%	0.057%
9	5.028	278	279	283	rVB2	1651	1599	0.18%	0.016%
10	5.310	323	327	328	rVV3	2344	2222	0.24%	0.022%
11	5.856	418	420	425	rVB2	1539	1884	0.21%	0.018%
12	5.968	437	439	442	rBV2	1601	1856	0.20%	0.018%
13	6.232	481	484	488	rVB2	1035	1767	0.19%	0.017%
14	7.413	677	685	694	rVB	136108	231348	25.35%	2.254%
15	7.613	713	719	727	rBV	118419	188645	20.67%	1.838%
16	7.742	739	741	746	rBV	1082	1662	0.18%	0.016%
17	7.807	746	752	757	rBV	129805	222757	24.41%	2.170%
18	7.965	775	779	783	rBV	1214	2235	0.24%	0.022%
19	8.171	810	814	816	rBV2	1280	1604	0.18%	0.016%
20	8.294	829	835	842	rBV	95779	159149	17.44%	1.550%
21	8.976	943	951	959	rBV2	175931	298344	32.69%	2.906%
22	9.493	1030	1039	1046	rBV	147711	262830	28.80%	2.560%
23	9.599	1051	1057	1058	rBV2	2730	3099	0.34%	0.030%
24	10.210	1153	1161	1171	rBV2	117188	215568	23.62%	2.100%
25	10.733	1243	1250	1258	rVB2	178542	315724	34.59%	3.076%
26	11.138	1312	1319	1328	rVB	154587	272324	29.84%	2.653%
27	11.279	1336	1343	1351	rBV	182260	334615	36.66%	3.260%
28	12.695	1579	1584	1588	rVB3	3432	5002	0.55%	0.049%
29	13.183	1664	1667	1670	rBV2	1468	1740	0.19%	0.017%
30	13.253	1677	1679	1684	rVB	1813	2011	0.22%	0.020%
31	13.406	1702	1705	1709	rVB	1607	1980	0.22%	0.019%
32	13.494	1716	1720	1725	rVB2	2517	3095	0.34%	0.030%
33	13.594	1732	1737	1740	rBV2	874	1614	0.18%	0.016%
34	13.670	1748	1750	1757	rVB	1717	2058	0.23%	0.020%
35	13.753	1757	1764	1771	rBV	77940	116423	12.76%	1.134%
36	14.093	1817	1822	1828	rBV6	4885	9871	1.08%	0.096%

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37	14.317	1854	1860	1866	rBV	359910	499256	54.70%	4.863%
38	14.505	1888	1892	1899	rBV3	1712	3848	0.42%	0.037%
39	14.628	1906	1913	1922	rVB	410308	656259	71.90%	6.393%
40	14.834	1945	1948	1954	rBV2	3012	4553	0.50%	0.044%
41	14.922	1957	1963	1969	rVV2	235319	376512	41.25%	3.668%
42	15.092	1982	1992	1997	rBV	87962	139354	15.27%	1.357%
43	15.257	2015	2020	2024	rBV2	3111	4896	0.54%	0.048%
44	15.909	2123	2131	2138	rBV	534756	799914	87.64%	7.792%
45	16.015	2143	2149	2155	rVV	100256	146816	16.09%	1.430%
46	16.150	2169	2172	2176	rVB2	2001	2637	0.29%	0.026%
47	16.696	2261	2265	2270	rBV3	2305	5109	0.56%	0.050%
48	16.884	2292	2297	2302	rBV3	4964	7313	0.80%	0.071%
49	16.990	2309	2315	2319	rBV4	5625	9252	1.01%	0.090%
50	17.084	2328	2331	2334	rBV	1529	2083	0.23%	0.020%
51	17.337	2370	2374	2375	rBV	2086	1848	0.20%	0.018%
52	17.413	2385	2387	2390	rVB	1644	1662	0.18%	0.016%
53	17.448	2390	2393	2394	rBV	1906	1696	0.19%	0.017%
54	17.507	2398	2403	2406	rVV3	5516	8579	0.94%	0.084%
55	17.548	2409	2410	2415	rVB2	1766	1761	0.19%	0.017%
56	17.672	2425	2431	2438	rVB	298067	446471	48.92%	4.349%
57	17.771	2441	2448	2455	rVV2	544434	822084	90.07%	8.008%
58	17.824	2455	2457	2462	rVV6	5952	7383	0.81%	0.072%
59	17.907	2466	2471	2473	rVV4	2607	3418	0.37%	0.033%
60	17.924	2473	2474	2478	rVB4	2275	1645	0.18%	0.016%
61	18.271	2529	2533	2538	rVB3	9143	10622	1.16%	0.103%
62	18.371	2548	2550	2554	rBV2	3319	3184	0.35%	0.031%
63	18.435	2560	2561	2563	rBV2	2880	1903	0.21%	0.019%
64	18.488	2566	2570	2581	rBV	77312	118334	12.97%	1.153%
65	18.588	2584	2587	2590	rVB3	5481	6641	0.73%	0.065%
66	18.764	2614	2617	2620	rBV3	3515	5227	0.57%	0.051%
67	18.905	2639	2641	2643	rVB2	2940	2334	0.26%	0.023%
68	19.135	2676	2680	2681	rBV2	2557	2351	0.26%	0.023%
69	19.164	2683	2685	2689	rVB4	2419	2189	0.24%	0.021%
70	19.364	2716	2719	2721	rBV3	1737	2172	0.24%	0.021%
71	19.393	2721	2724	2727	rVV4	6513	8143	0.89%	0.079%
72	19.428	2727	2730	2738	rVB2	19618	23307	2.55%	0.227%
73	19.558	2746	2752	2756	rBV7	3937	5959	0.65%	0.058%
74	19.610	2757	2761	2764	rBV4	10375	14730	1.61%	0.143%
75	19.751	2781	2785	2789	rBV4	15659	24882	2.73%	0.242%
76	19.963	2817	2821	2826	rVB5	6910	9998	1.10%	0.097%

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77	20.045	2826	2835	2842	rBV	635448	911308	99.85%	8.877%
78	20.274	2871	2874	2876	rBV3	2866	3294	0.36%	0.032%
79	20.486	2908	2910	2915	rVB3	8902	8105	0.89%	0.079%
80	21.361	3055	3059	3066	rVB3	22540	31927	3.50%	0.311%
81	21.432	3066	3071	3078	rBV2	47410	74629	8.18%	0.727%
82	21.543	3086	3090	3105	rVB4	23406	59663	6.54%	0.581%
83	21.990	3160	3166	3173	rVB	256834	428613	46.96%	4.175%
84	22.578	3265	3266	3270	rVB4	4533	3422	0.37%	0.033%
85	22.760	3293	3297	3300	rBV5	11276	16795	1.84%	0.164%
86	23.858	3482	3484	3485	rBV2	4626	3205	0.35%	0.031%
87	24.387	3570	3574	3581	rVB4	26451	54239	5.94%	0.528%
88	25.286	3716	3727	3741	rBV3	309524	912692	100.00%	8.891%
89	25.533	3760	3769	3783	rVB2	152321	474026	51.94%	4.618%
90	25.809	3815	3816	3818	rBV2	3993	1889	0.21%	0.018%
91	26.367	3909	3911	3912	rBV2	6505	3379	0.37%	0.033%
92	26.690	3960	3966	3982	rVB4	23192	74451	8.16%	0.725%
93	26.902	4000	4002	4003	rBV2	5083	3309	0.36%	0.032%
94	27.348	4076	4078	4079	rBV2	3848	2722	0.30%	0.027%
95	28.183	4216	4220	4222	rBV4	11893	17028	1.87%	0.166%
96	30.850	4672	4674	4675	rBV2	4454	2219	0.24%	0.022%
97	31.450	4775	4776	4778	rVB2	5143	2721	0.30%	0.027%
98	31.549	4791	4793	4795	rBV3	3839	2796	0.31%	0.027%
99	31.843	4841	4843	4844	rBV	3464	2759	0.30%	0.027%
100	32.501	4954	4955	4959	rVB3	4060	2605	0.29%	0.025%

Sum of corrected areas: 10265607

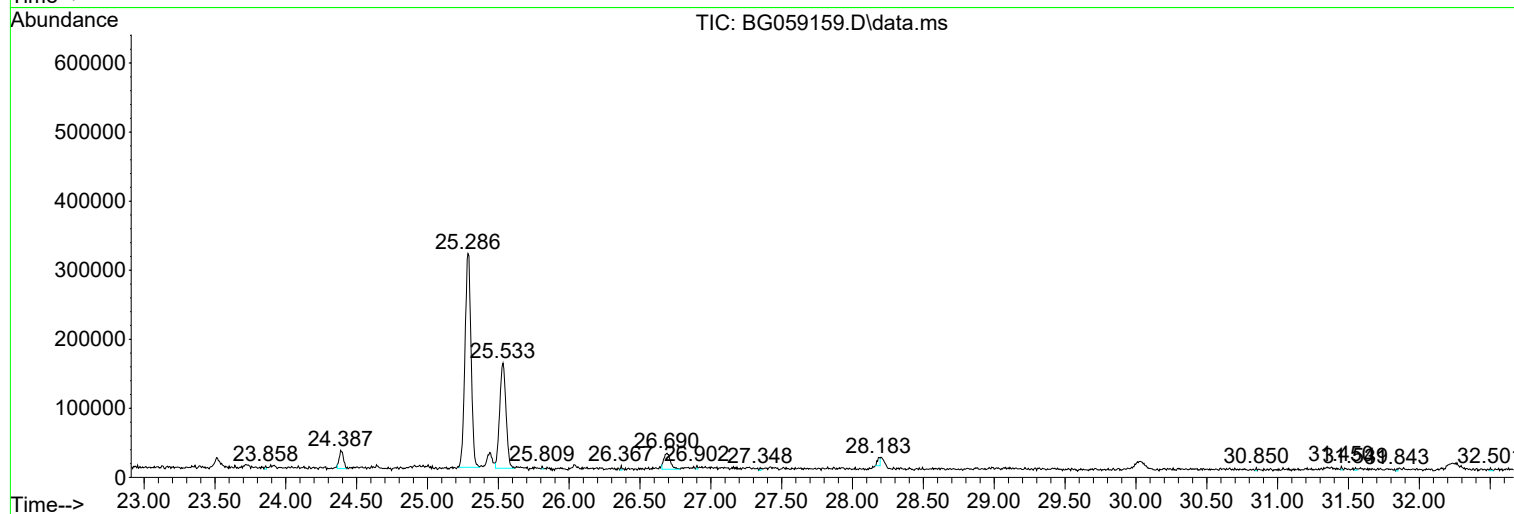
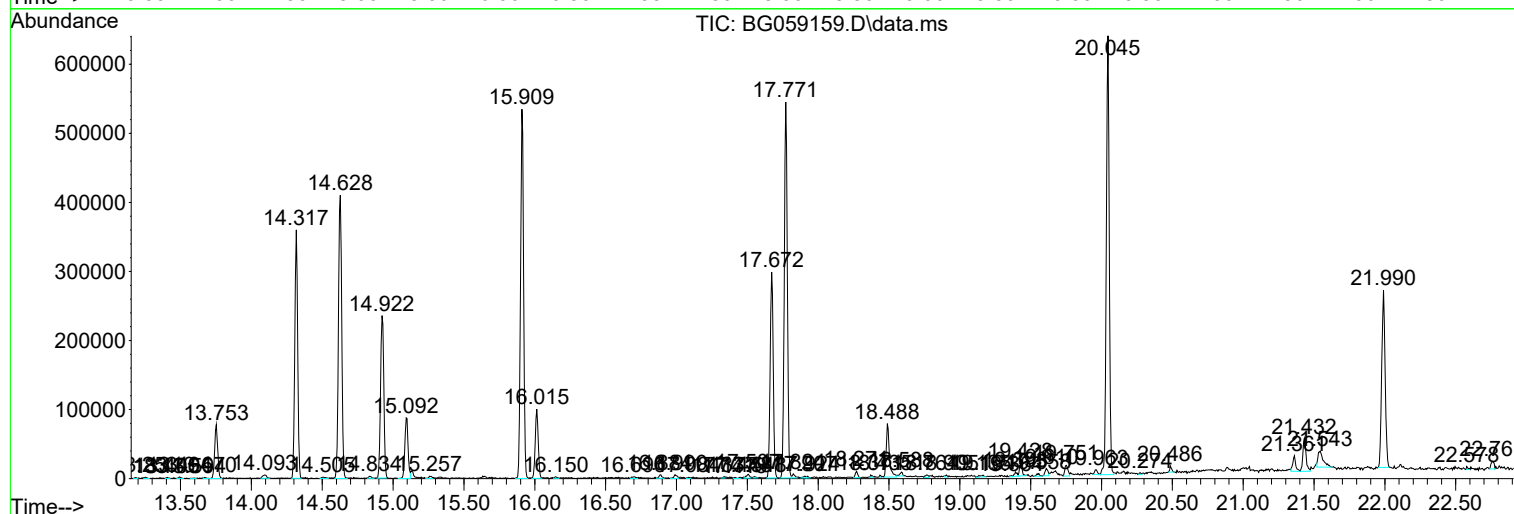
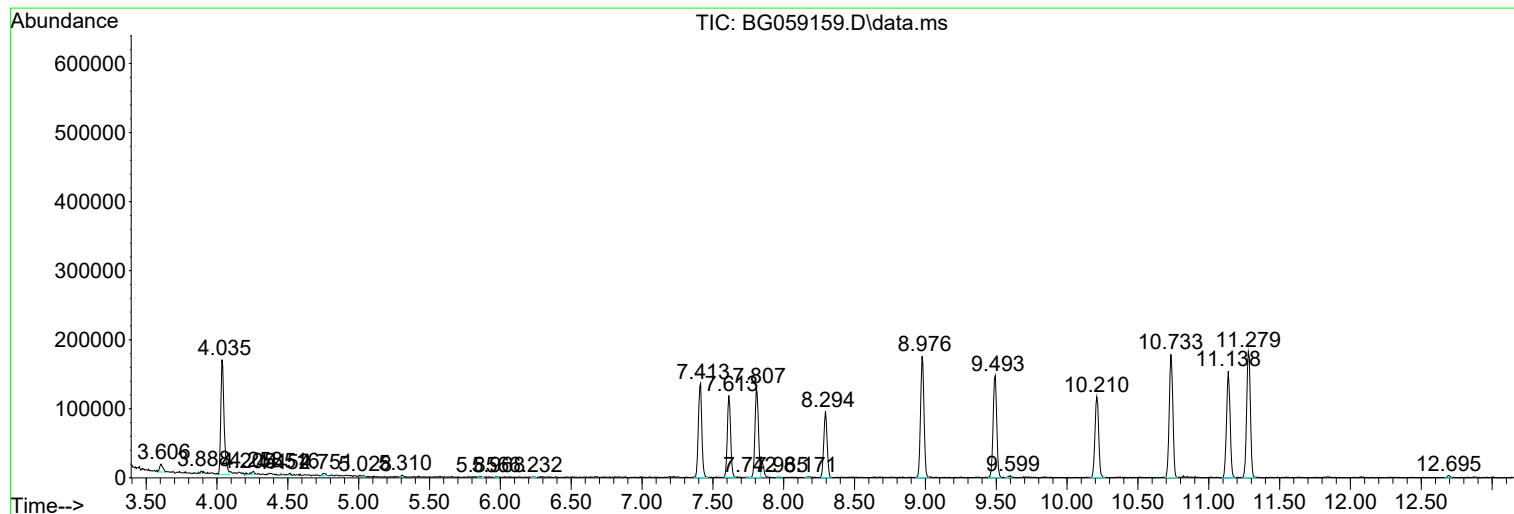
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L

TIC Integration Parameters: LSCINT.P



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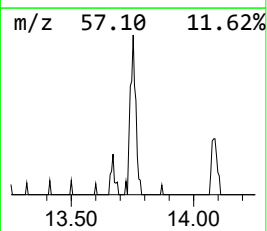
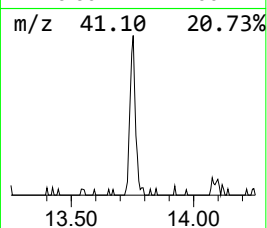
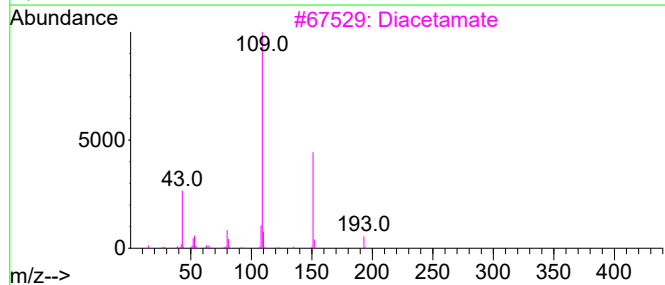
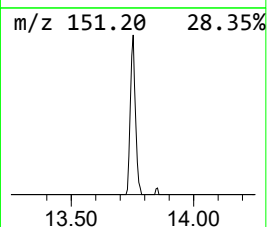
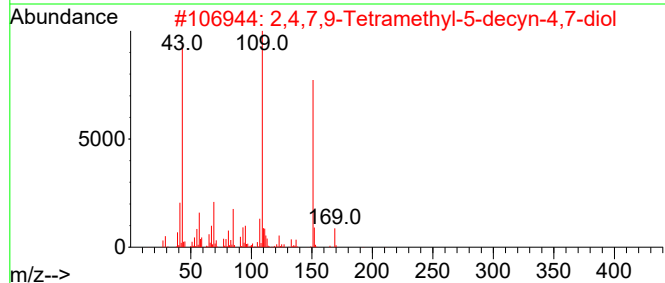
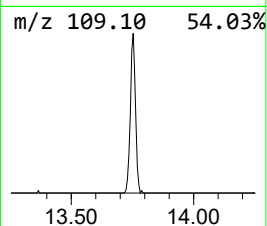
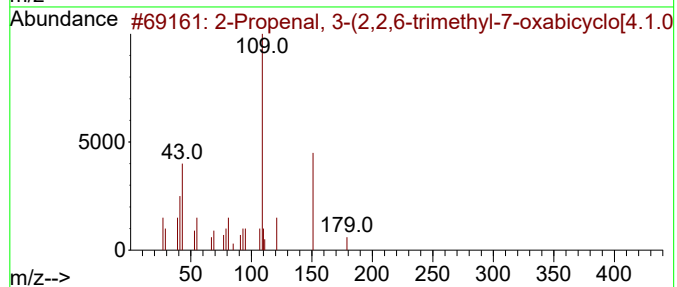
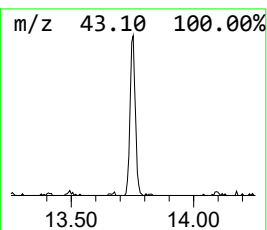
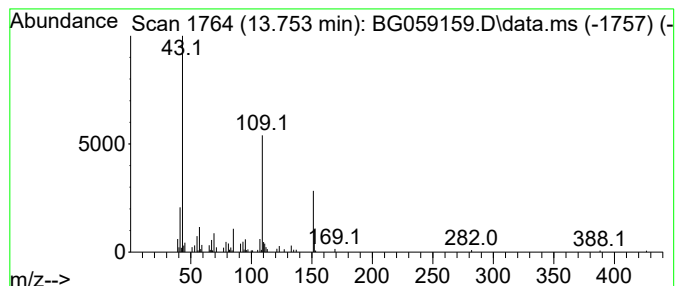
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091923.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 2-Propenal, 3-(2,2,6-trimet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.753	6.18 ng/ul	116423	Acenaphthene-d10	14.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	59	
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	53	
3	Diacetamate	193	C10H11NO3	002623-33-8	50	
4	Metacetamol	151	C8H9NO2	000621-42-1	50	
5	Acetaminophen	151	C8H9NO2	000103-90-2	50	



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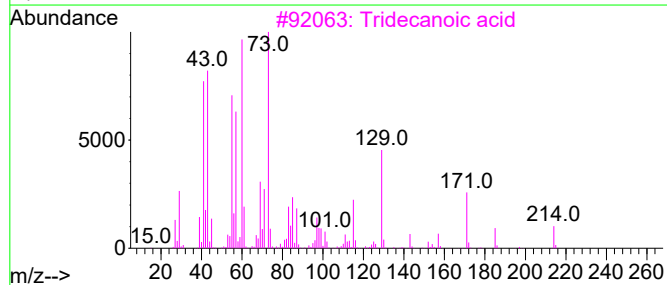
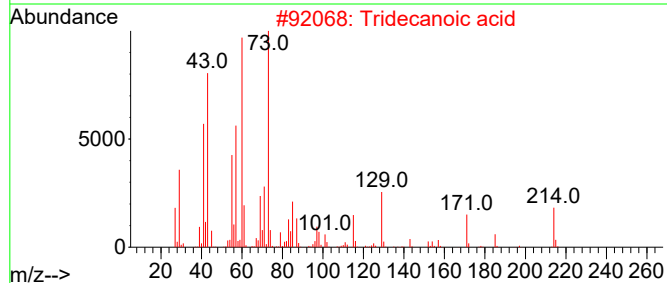
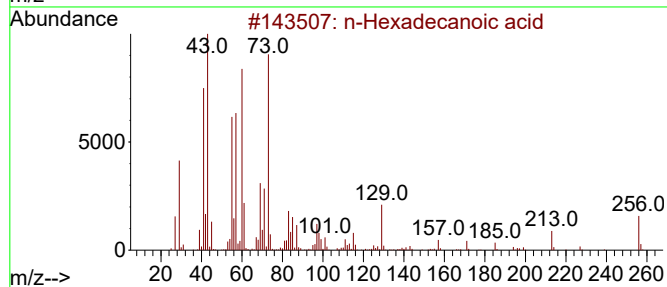
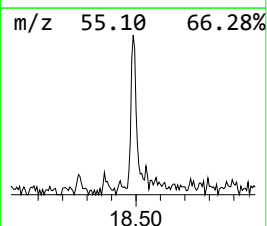
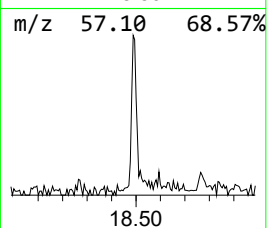
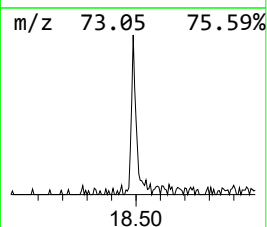
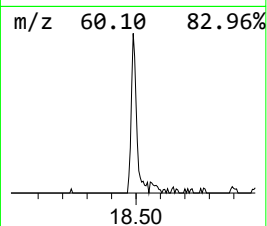
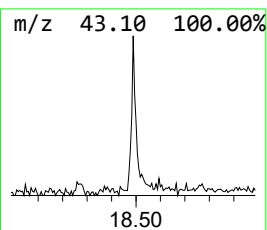
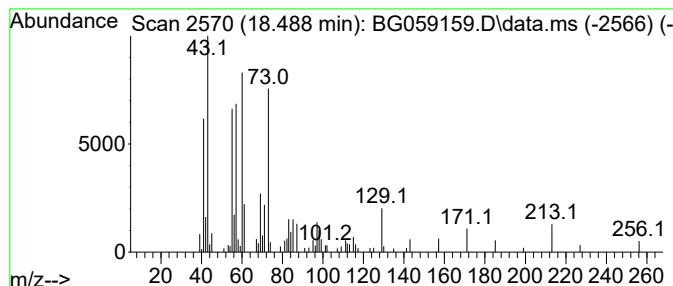
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.488	5.30 ng/ul	118334	Phenanthrene-d10	17.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Tridecanoic acid	214	C13H26O2	000638-53-9	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



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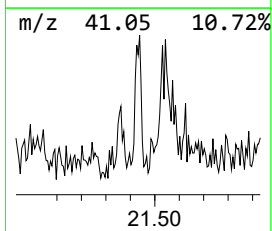
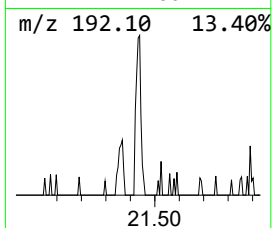
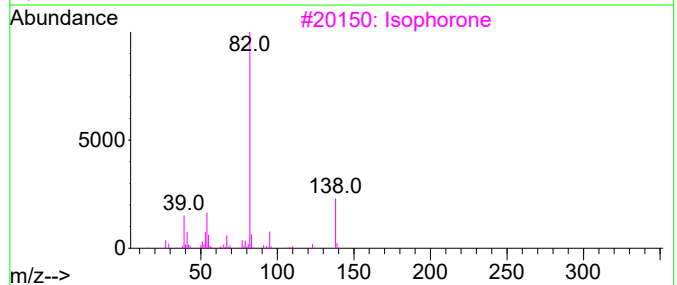
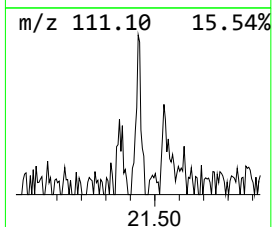
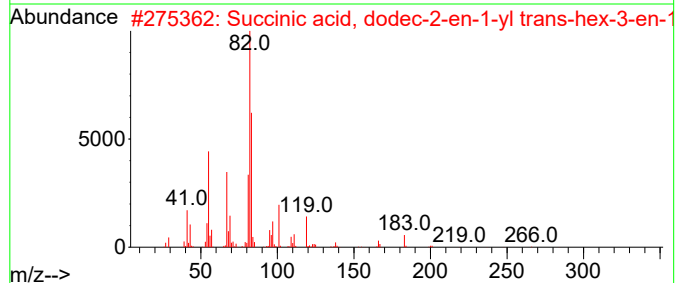
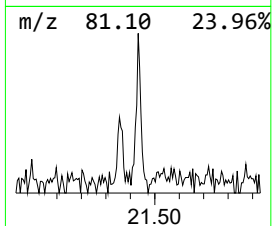
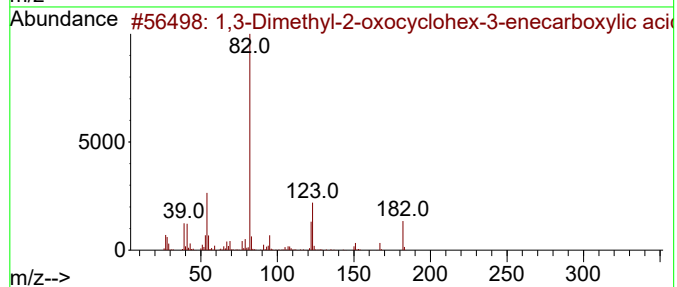
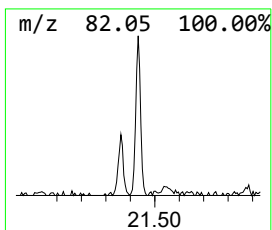
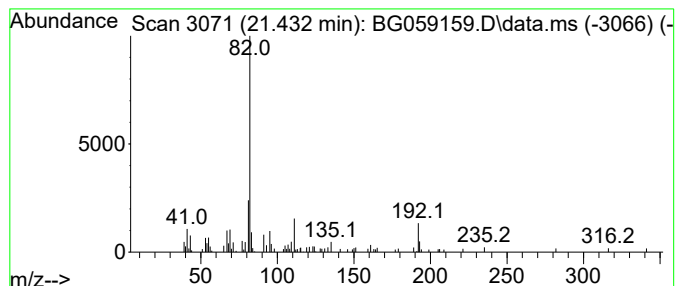
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091923.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 1,3-Dimethyl-2-oxocyclohex-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.432	3.48 ng/ul	74629	Chrysene-d12	21.990

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dimethyl-2-oxocyclohex-3-ene...	182	C10H14O3	1000211-14-8	53
2			Succinic acid, dodec-2-en-1-yl t...	366	C22H38O4	1000391-12-5	45
3			Isophorone	138	C9H14O	000078-59-1	42
4			Pyrazole-3-propanoic acid, .beta...	253	C12H19N3O3	1010269-45-3	42
5			Isophorone	138	C9H14O	000078-59-1	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092023\
Data File : BG059159.D
Acq On : 22 Sep 2023 11:07
Operator : MA/JU
Sample : 04386-14
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AM9

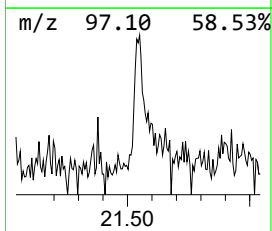
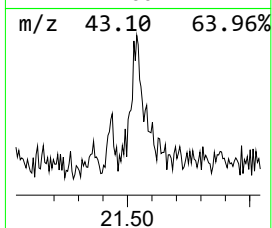
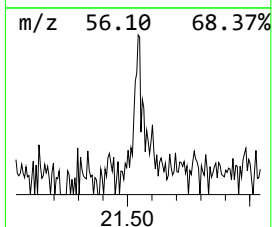
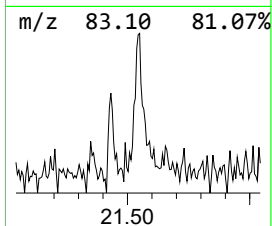
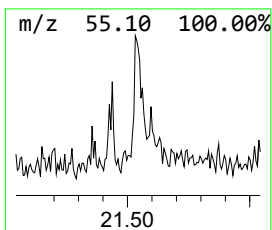
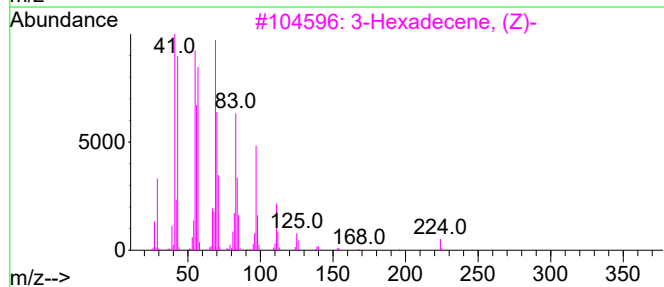
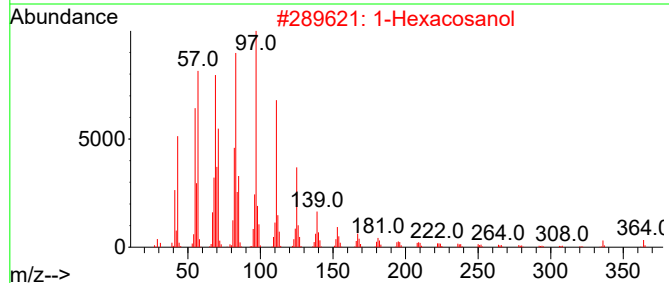
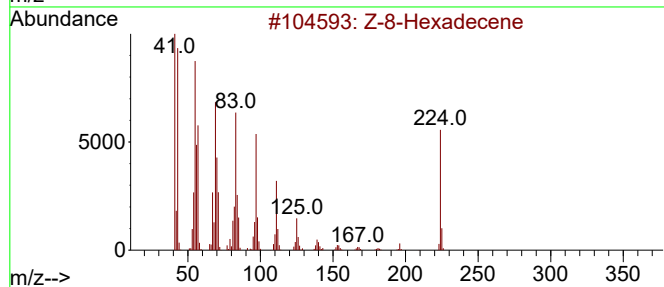
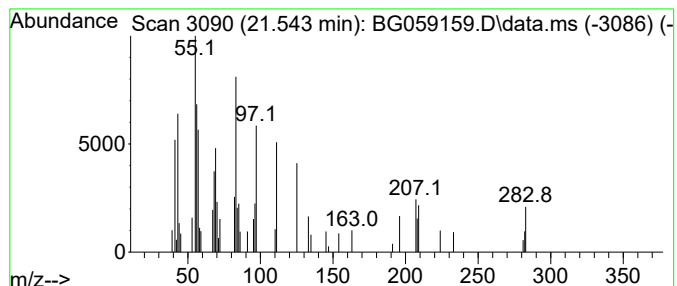
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.544	2.78 ng/ul	59663	Chrysene-d12	21.990

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Z-8-Hexadecene	224	C16H32	1000130-87-5	47
2			1-Hexacosanol	382	C26H54O	000506-52-5	43
3			3-Hexadecene, (Z)-	224	C16H32	034303-81-6	43
4			3-Chloropropionic acid, octadecy...	360	C21H41ClO2	088168-99-4	38
5			Triacontan-15-ol	438	C30H62O	031849-26-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092023\
Data File : BG059159.D
Acq On : 22 Sep 2023 11:07
Operator : MA/JU
Sample : 04386-14
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AM9

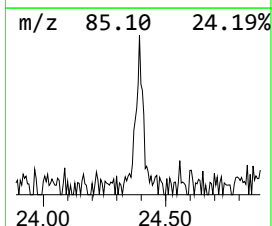
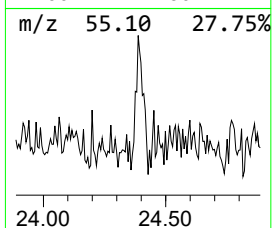
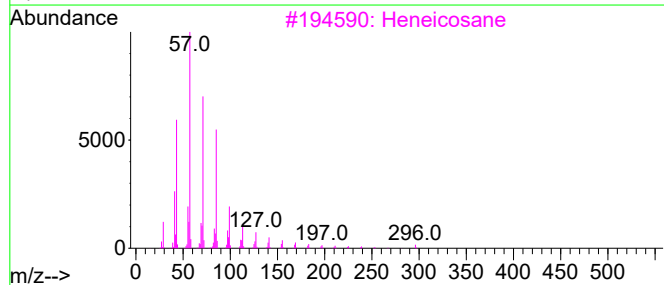
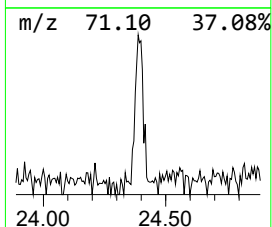
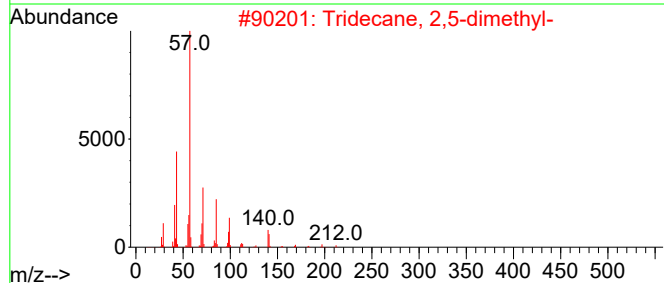
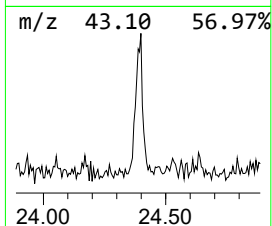
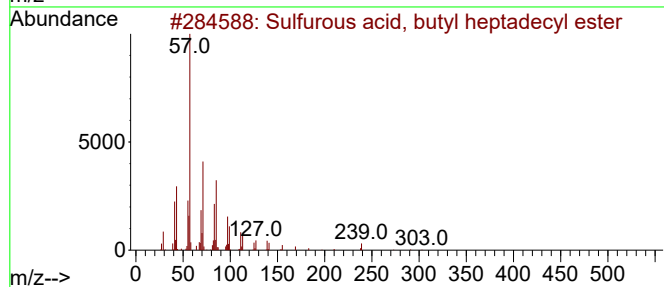
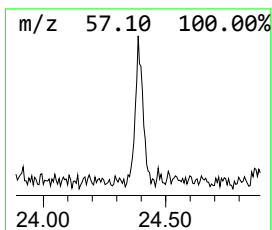
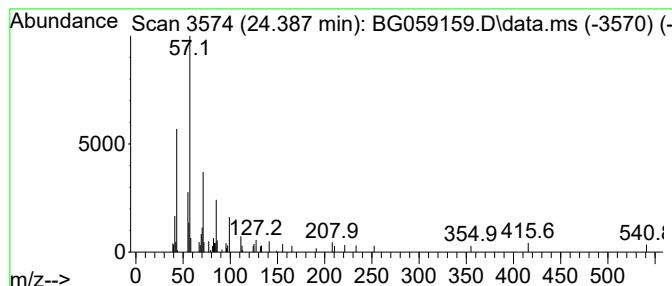
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Sulfurous acid, butyl hepta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.387	2.29 ng/ul	54239	Perylene-d12	25.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	59
2			Tridecane, 2,5-dimethyl-	212	C15H32	056292-66-1	59
3			Heneicosane	296	C21H44	000629-94-7	53
4			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	53
5			Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092023\
Data File : BG059159.D
Acq On : 22 Sep 2023 11:07
Operator : MA/JU
Sample : 04386-14
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AM9

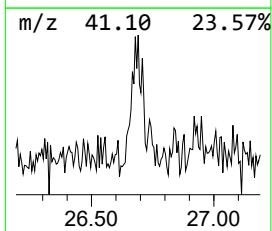
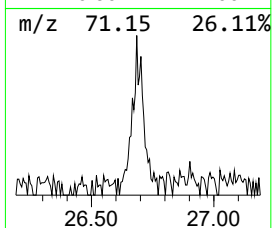
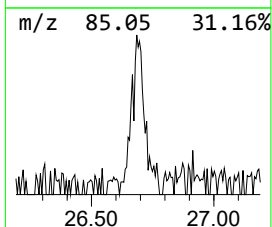
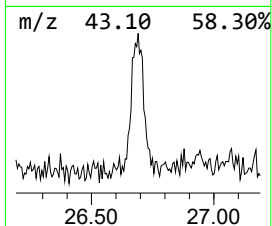
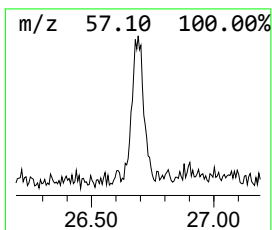
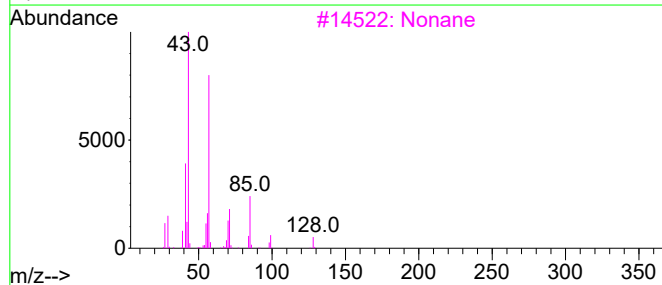
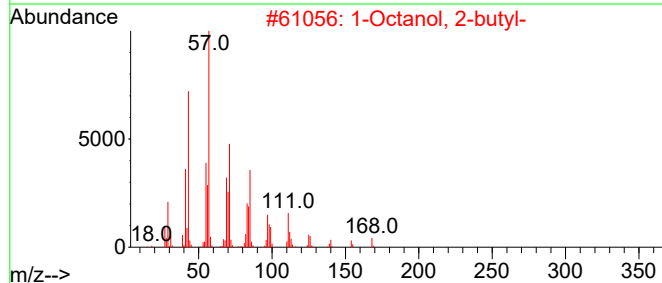
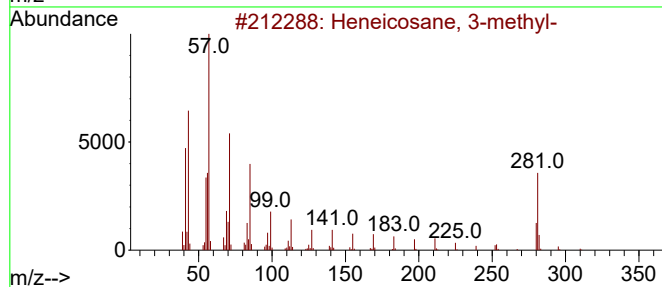
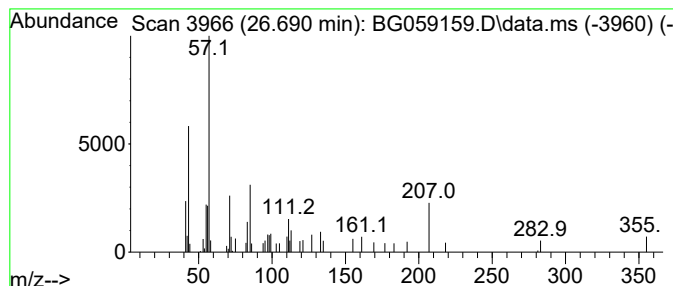
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091923.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.690	3.14 ng/ul	74451	Perylene-d12	25.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane, 3-methyl-	310	C22H46	006418-47-9	43
2			1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	43
3			Nonane	128	C9H20	000111-84-2	43
4			1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	38
5			Nonane	128	C9H20	000111-84-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG092023\
Data File : BG059159.D
Acq On : 22 Sep 2023 11:07
Operator : MA/JU
Sample : 04386-14
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0AM9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG091923.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
2-Propenal, 3-(...	13.753	6.2	ng/ul	116423	3	14.922	376512	20.0
n-Hexadecanoic ...	18.488	5.3	ng/ul	118334	4	17.672	446471	20.0
1,3-Dimethyl-2-...	21.432	3.5	ng/ul	74629	5	21.990	428613	20.0
(DEL) Alkane: S...	21.544	2.8	ng/ul	59663	5	21.990	428613	20.0
Sulfurous acid,...	24.387	2.3	ng/ul	54239	6	25.533	474026	20.0
(DEL) Alkane: S...	26.690	3.1	ng/ul	74451	6	25.533	474026	20.0