

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100723\
 Data File : BG059352.D
 Acq On : 7 Oct 2023 21:35
 Operator : MA/JU
 Sample : 04607-19
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BBHA7

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-BG100723.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG059352.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.491	10	17	35	rBV	3904200	6751194	100.00%	27.179%
2	3.967	92	98	108	rBV	58176	97727	1.45%	0.393%
3	4.830	239	245	253	rBV8	10064	16254	0.24%	0.065%
4	7.351	668	674	681	rBV	45765	83457	1.24%	0.336%
5	7.551	700	708	717	rBV	177723	301507	4.47%	1.214%
6	7.745	733	741	748	rBV	167287	288808	4.28%	1.163%
7	8.232	817	824	829	rBV	136878	230092	3.41%	0.926%
8	8.920	931	941	948	rBV2	139910	253596	3.76%	1.021%
9	8.990	948	953	958	rVV2	12696	27016	0.40%	0.109%
10	9.043	958	962	965	rVV4	5411	9851	0.15%	0.040%
11	9.078	965	968	974	rVB3	4045	6801	0.10%	0.027%
12	9.425	1017	1027	1035	rBV	235162	406364	6.02%	1.636%
13	9.631	1058	1062	1064	rBV4	4538	7617	0.11%	0.031%
14	9.783	1083	1088	1090	rBV3	7782	11421	0.17%	0.046%
15	10.142	1140	1149	1156	rBV	171822	316847	4.69%	1.276%
16	10.201	1156	1159	1163	rVB4	7040	11096	0.16%	0.045%
17	10.553	1218	1219	1224	rVB3	7768	8314	0.12%	0.033%
18	10.671	1232	1239	1247	rBV2	262725	494209	7.32%	1.990%
19	10.941	1279	1285	1291	rVB5	11013	20443	0.30%	0.082%
20	11.070	1299	1307	1313	rBV	207303	381915	5.66%	1.538%
21	11.123	1313	1316	1324	rVB4	8282	16330	0.24%	0.066%
22	11.217	1324	1332	1341	rBV2	271738	508804	7.54%	2.048%
23	11.699	1412	1414	1418	rVV4	6522	7562	0.11%	0.030%
24	11.822	1432	1435	1442	rVB7	4299	9013	0.13%	0.036%
25	11.987	1459	1463	1465	rVB4	8706	10884	0.16%	0.044%
26	12.868	1605	1613	1616	rBV8	4912	11351	0.17%	0.046%
27	13.691	1748	1753	1758	rBV	32855	50938	0.75%	0.205%
28	14.260	1842	1850	1856	rVV	647792	940789	13.94%	3.787%
29	14.566	1895	1902	1910	rBV	737364	1123029	16.63%	4.521%
30	14.860	1945	1952	1959	rBV	358665	573532	8.50%	2.309%
31	15.054	1979	1985	1993	rBV	56595	98661	1.46%	0.397%
32	15.853	2114	2121	2128	rBV	985866	1506360	22.31%	6.064%
33	15.964	2133	2140	2146	rVV	388409	551745	8.17%	2.221%
34	16.094	2156	2162	2170	rVB4	26835	50656	0.75%	0.204%
35	16.470	2223	2226	2230	rVB6	4735	6831	0.10%	0.028%
36	17.081	2325	2330	2335	rBV3	44384	60037	0.89%	0.242%

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Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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37	17.280	2359	2364	2368	rBV3	5342	7707	0.11%	0.031%
38	17.316	2368	2370	2376	rVB3	7864	8829	0.13%	0.036%
39	17.609	2414	2420	2427	rBV	494697	756582	11.21%	3.046%
40	17.709	2431	2437	2446	rVB2	1153305	1739472	25.77%	7.003%
41	17.991	2482	2485	2488	rBV3	5968	7302	0.11%	0.029%
42	18.432	2555	2560	2565	rBV3	38621	59260	0.88%	0.239%
43	18.520	2574	2575	2580	rVB2	7947	8566	0.13%	0.034%
44	18.779	2617	2619	2622	rBV4	7844	10273	0.15%	0.041%
45	19.554	2746	2751	2755	rVV7	20866	35244	0.52%	0.142%
46	19.613	2755	2761	2765	rVB4	17682	31975	0.47%	0.129%
47	19.689	2771	2774	2781	rVB6	27747	38783	0.57%	0.156%
48	19.789	2789	2791	2794	rBV4	6477	7108	0.11%	0.029%
49	19.830	2796	2798	2802	rVB5	9335	12682	0.19%	0.051%
50	19.989	2819	2825	2833	rVV	1397570	2018881	29.90%	8.128%
51	20.118	2845	2847	2850	rBV4	5252	7704	0.11%	0.031%
52	20.870	2971	2975	2979	rVB7	10288	19799	0.29%	0.080%
53	20.917	2981	2983	2984	rBV2	7174	6987	0.10%	0.028%
54	21.053	3000	3006	3008	rBV7	19038	38221	0.57%	0.154%
55	21.452	3072	3074	3079	rBV6	7961	13512	0.20%	0.054%
56	21.575	3094	3095	3098	rBV3	8722	8130	0.12%	0.033%
57	21.628	3102	3104	3106	rBV3	7455	8502	0.13%	0.034%
58	21.716	3116	3119	3125	rVB4	19918	28963	0.43%	0.117%
59	21.916	3146	3153	3159	rVV	459742	787499	11.66%	3.170%
60	22.010	3167	3169	3174	rBV6	7963	12701	0.19%	0.051%
61	22.651	3276	3278	3279	rBV2	9511	7801	0.12%	0.031%
62	22.704	3284	3287	3288	rBV3	7899	9109	0.13%	0.037%
63	23.009	3337	3339	3343	rVV5	15852	18565	0.27%	0.075%
64	23.080	3347	3351	3356	rVB7	25580	40345	0.60%	0.162%
65	23.391	3398	3404	3410	rBV6	29978	69521	1.03%	0.280%
66	24.255	3545	3551	3556	rVB6	36568	69597	1.03%	0.280%
67	25.159	3693	3705	3714	rVV2	718885	2140236	31.70%	8.616%
68	25.259	3717	3722	3731	rVB5	52852	141801	2.10%	0.571%
69	25.400	3736	3746	3760	rVB3	294224	917739	13.59%	3.695%
70	26.335	3903	3905	3907	rBV3	6601	6942	0.10%	0.028%
71	26.487	3920	3931	3940	rBV3	47620	164729	2.44%	0.663%
72	26.775	3978	3980	3983	rBV4	5683	7692	0.11%	0.031%
73	27.944	4171	4179	4191	rVB3	45440	155628	2.31%	0.627%
74	28.879	4335	4338	4339	rBV3	6917	7959	0.12%	0.032%
75	29.037	4363	4365	4372	rVB8	8487	12092	0.18%	0.049%
76	29.713	4472	4480	4486	rVV9	27644	91213	1.35%	0.367%

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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

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77	30.500	4612	4614	4617	rVB4	7425	8433	0.12%	0.034%
78	31.205	4733	4734	4739	rBV5	6013	8288	0.12%	0.033%
79	31.252	4739	4742	4743	rBV3	9362	7157	0.11%	0.029%
80	31.846	4840	4843	4844	rBV2	17739	19109	0.28%	0.077%
81	32.051	4875	4878	4880	rBV4	10289	9937	0.15%	0.040%

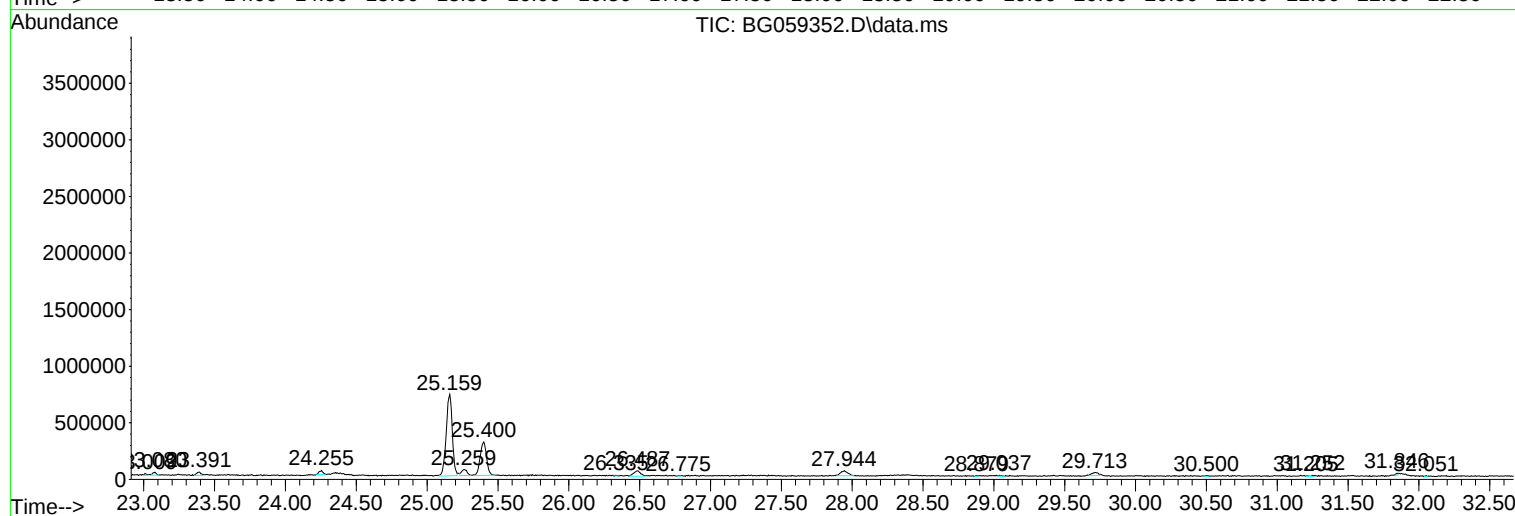
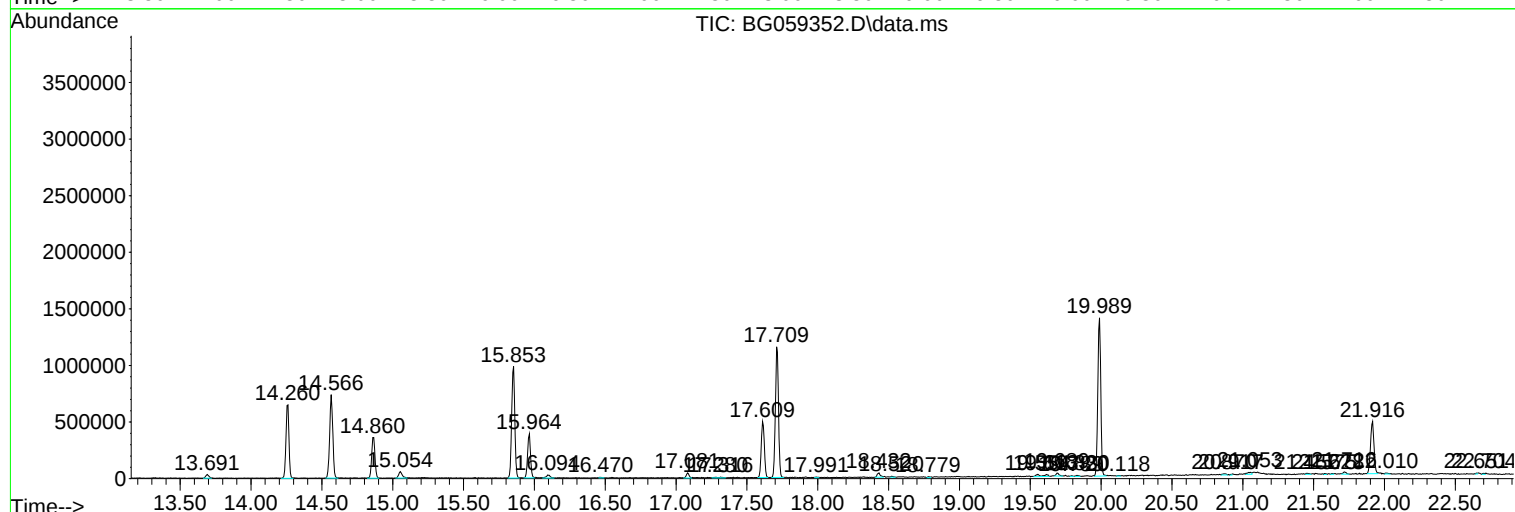
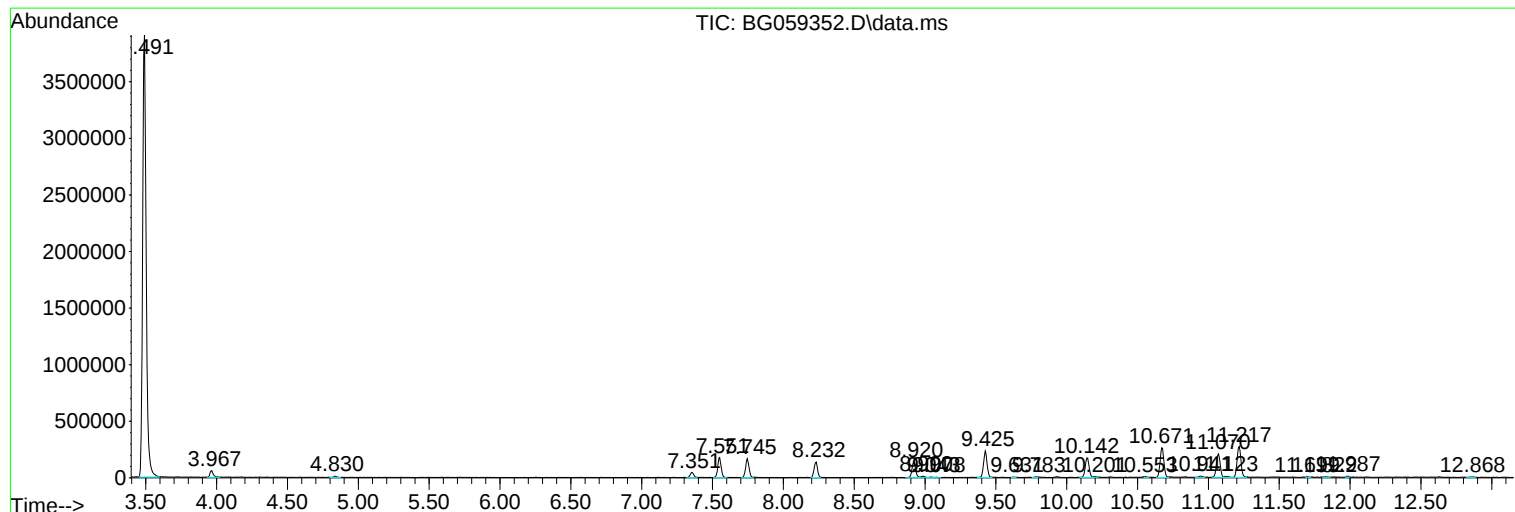
Sum of corrected areas: 24839626

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG100723.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\BG100723\
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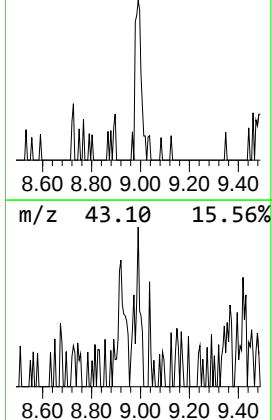
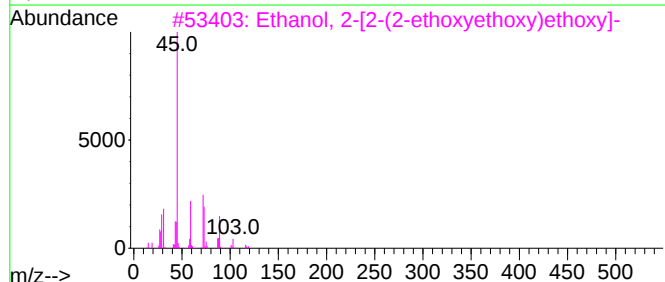
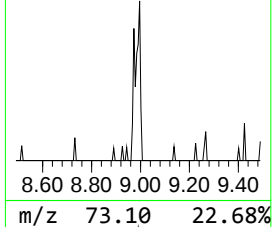
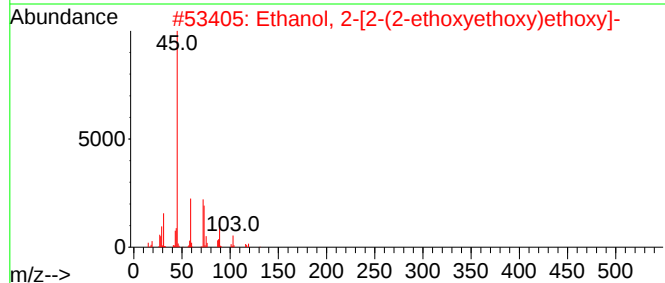
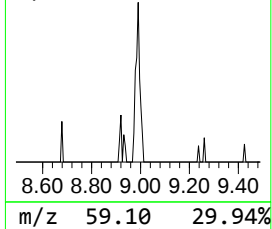
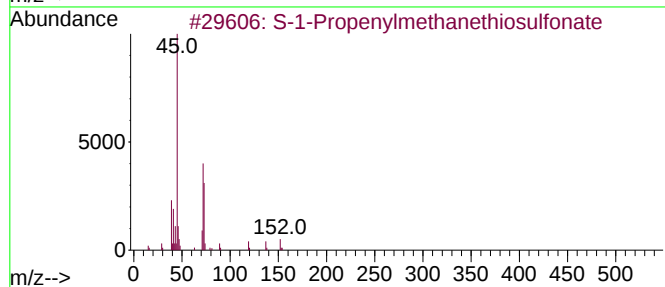
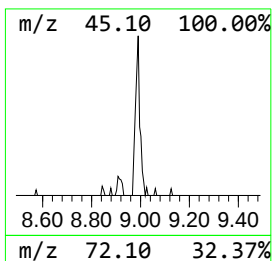
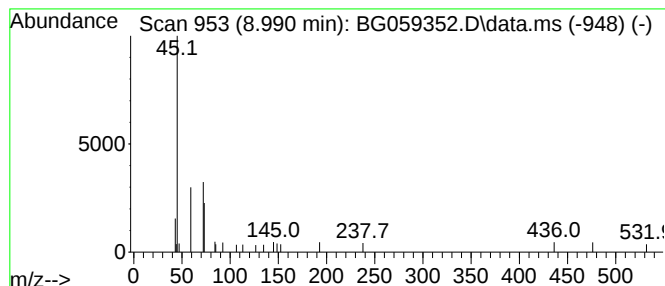
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG100723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 S-1-Propenylmethanethiosulf... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.990	2.35 ng/ul	27016	1,4-Dichlorobenzene-d4	8.226	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-1-Propenylmethanethiosulfonate	152	C4H8O2S2	1000322-28-8	53
2	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50
4	1-(2-Hydroxyethoxy)-2-(vinylthio...	148	C6H12O2S	086241-10-3	28
5	1-Bromo-7-octanol	208	C8H17BrO	126680-20-4	9



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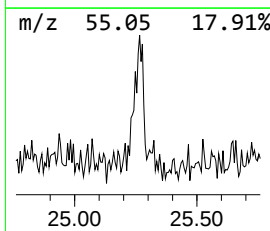
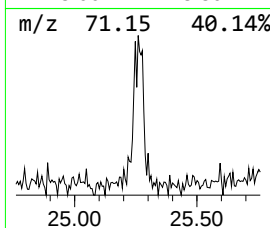
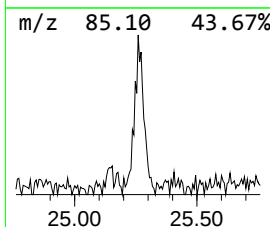
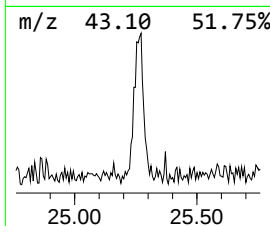
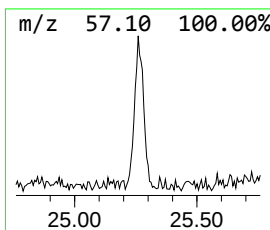
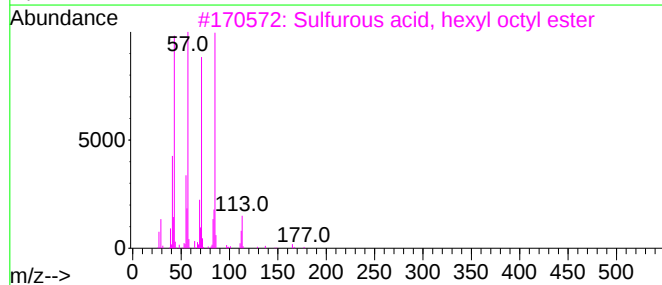
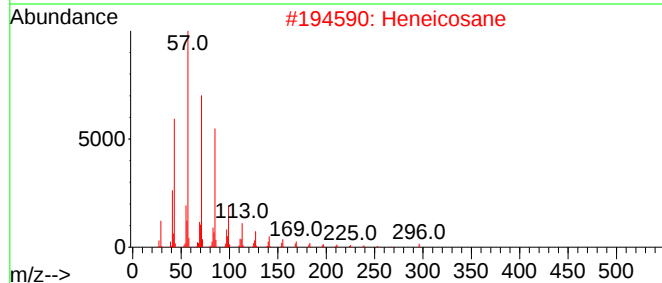
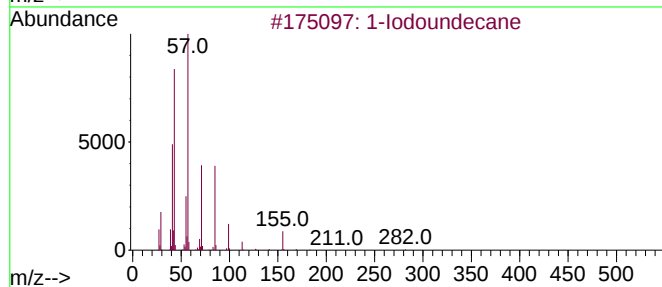
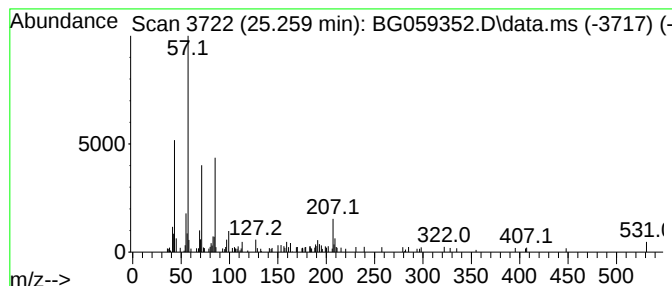
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG100723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 1-Iodoundecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.259	3.09 ng/ul	141801	Perylene-d12	25.400

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodoundecane			282	C11H23I	004282-44-4	53
2	Heneicosane			296	C21H44	000629-94-7	52
3	Sulfurous acid, hexyl octyl ester			278	C14H30O3S	1000309-13-0	50
4	Sulfurous acid, butyl heptadecyl...			376	C21H44O3S	1000309-18-4	50
5	Eicosane			282	C20H42	000112-95-8	49



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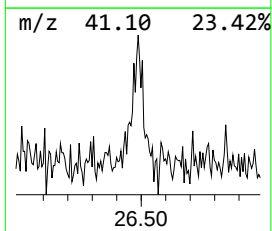
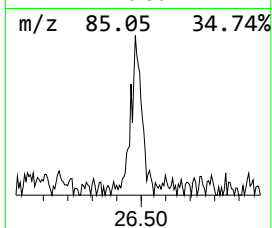
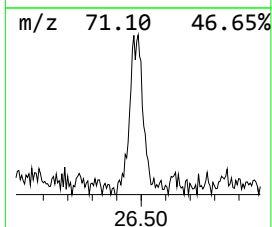
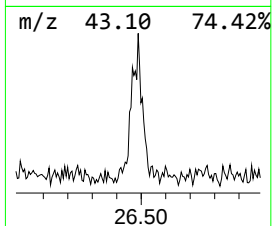
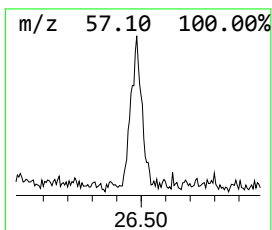
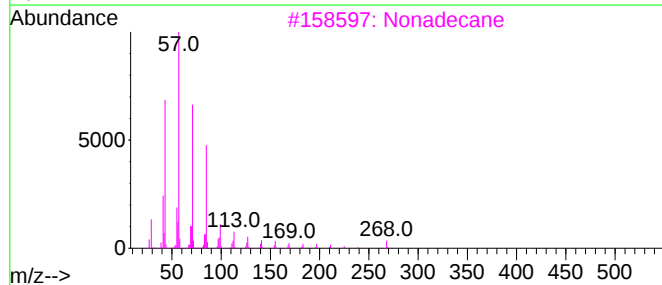
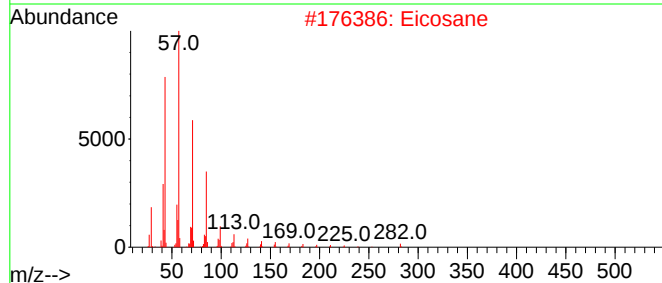
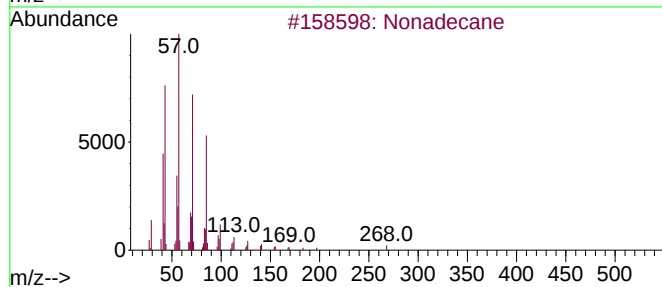
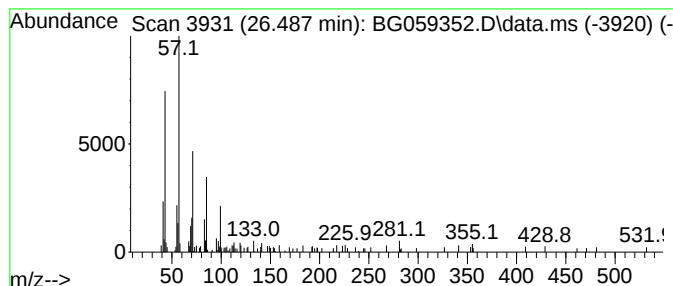
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG100723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.487	3.59 ng/ul	164729	Perylene-d12	25.400

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	64
2			Eicosane	282	C20H42	000112-95-8	58
3			Nonadecane	268	C19H40	000629-92-5	58
4			5-Ethylnonadecane	296	C21H44	1000360-43-1	53
5			Tetradecane	198	C14H30	000629-59-4	52



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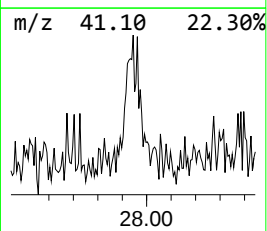
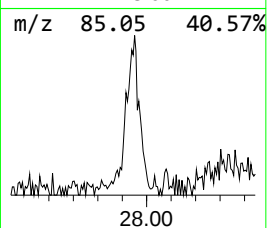
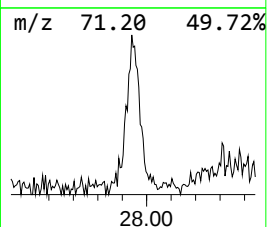
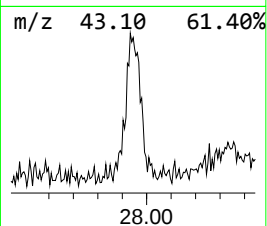
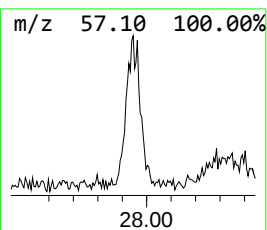
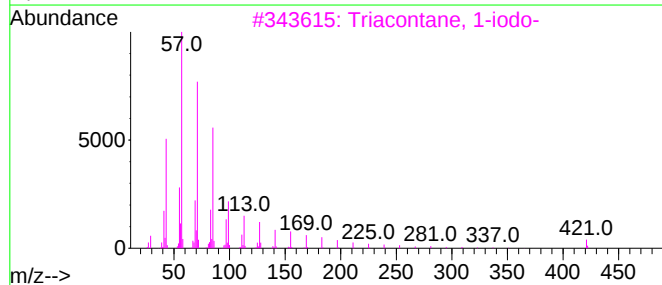
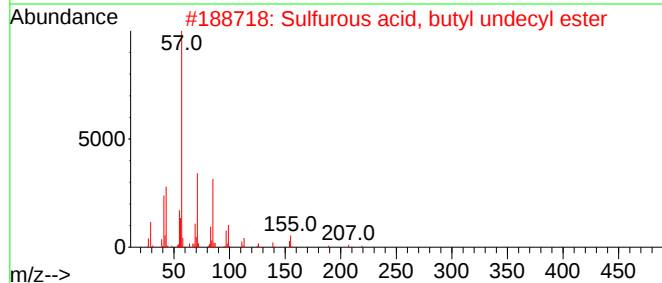
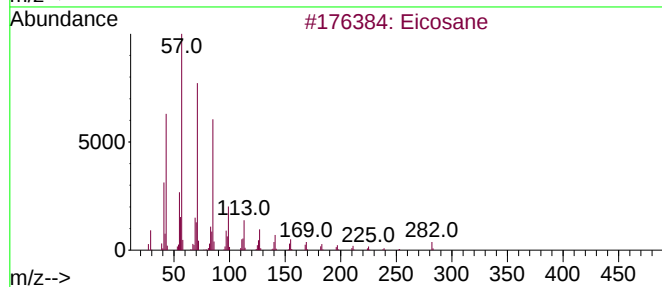
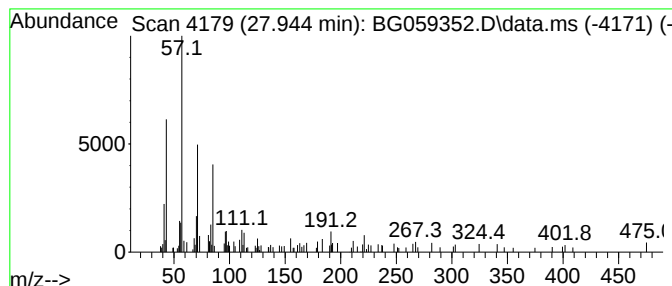
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.944	3.39 ng/ul	155628	Perylene-d12	25.400

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	62
2			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	58
3			Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	58
4			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	58
5			Hentriacontane	437	C31H64	000630-04-6	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100723\
Data File : BG059352.D
Acq On : 7 Oct 2023 21:35
Operator : MA/JU
Sample : 04607-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BBHA7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG100723.MA.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
S-1-Propenylmet...	8.990	2.4	ng/u1	27016	1	8.226	230092	20.0
1-Iodoundecane	25.259	3.1	ng/u1	141801	6	25.400	917739	20.0
(DEL) Alkane: S...	26.487	3.6	ng/u1	164729	6	25.400	917739	20.0
(DEL) Alkane: S...	27.944	3.4	ng/u1	155628	6	25.400	917739	20.0