

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040121\
 Data File : VV020858.D
 Acq On : 01 Apr 2021 23:33
 Operator : SY/MD
 Sample : M1845-10
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EW1B3

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M

Title : VOC Analysis

Signal : TIC: VV020849.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.311	76	84	95	rBV2	473450	501208	22.37%	2.268%
2	1.568	157	164	176	rBV	213442	238711	10.65%	1.080%
3	2.031	298	308	321	rBV	111733	168632	7.53%	0.763%
4	2.108	322	332	348	rBV	499031	740149	33.03%	3.350%
5	2.204	356	362	384	rVB	138412	226099	10.09%	1.023%
6	2.294	384	390	395	rBV2	3749	5240	0.23%	0.024%
7	2.433	423	433	464	rBV	667468	1224895	54.67%	5.543%
8	2.635	493	496	500	rVB6	1183	923	0.04%	0.004%
9	2.870	566	569	574	rBV4	1012	746	0.03%	0.003%
10	3.188	661	668	669	rBV4	895	803	0.04%	0.004%
11	3.227	678	680	685	rVB4	1015	738	0.03%	0.003%
12	3.381	724	728	731	rBV3	1110	941	0.04%	0.004%
13	3.609	796	799	802	rBV3	1026	738	0.03%	0.003%
14	3.764	843	847	848	rBV2	1106	627	0.03%	0.003%
15	3.812	849	862	877	rBV4	61893	150670	6.72%	0.682%
16	3.912	877	893	943	rVB2	485473	1476158	65.88%	6.681%
17	4.352	1013	1030	1057	rBV	397470	971726	43.37%	4.398%
18	4.513	1071	1080	1097	rBV2	27815	64173	2.86%	0.290%
19	4.796	1166	1168	1172	rVB3	1414	681	0.03%	0.003%
20	4.825	1174	1177	1183	rBV5	879	919	0.04%	0.004%
21	5.050	1230	1247	1280	rBV2	872649	2240647	100.00%	10.140%
22	5.349	1337	1340	1343	rBV3	840	637	0.03%	0.003%
23	5.416	1356	1361	1363	rBV4	1306	1264	0.06%	0.006%
24	5.561	1404	1406	1410	rVB5	1251	821	0.04%	0.004%
25	5.619	1410	1424	1443	rBV	680376	1419912	63.37%	6.426%
26	6.072	1552	1565	1588	rVB	485448	974320	43.48%	4.409%
27	6.613	1724	1733	1758	rBV2	88318	170251	7.60%	0.770%
28	6.767	1778	1781	1782	rBV4	1433	880	0.04%	0.004%
29	6.989	1839	1850	1872	rBV	287725	515838	23.02%	2.335%
30	7.095	1876	1883	1894	rVB6	6913	14369	0.64%	0.065%
31	7.320	1941	1953	1976	rBV	1047245	1797728	80.23%	8.136%
32	7.625	2037	2048	2066	rBV2	210349	369058	16.47%	1.670%
33	7.944	2140	2147	2151	rBV7	1188	2032	0.09%	0.009%
34	8.024	2161	2172	2181	rBV8	5483	10766	0.48%	0.049%
35	8.092	2183	2193	2227	rVV	592644	1069537	47.73%	4.840%
36	8.368	2268	2279	2280	rBV3	38971	57653	2.57%	0.261%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
 Title : VOC Analysis

37	8.715	2378	2387	2407	rVB2	50716	87074	3.89%	0.394%
38	8.857	2415	2431	2462	rBV	1074789	1813116	80.92%	8.206%
39	9.397	2595	2599	2606	rBV6	2828	3188	0.14%	0.014%
40	9.471	2619	2622	2623	rBV3	1916	1107	0.05%	0.005%
41	9.609	2660	2665	2668	rBV4	2674	2559	0.11%	0.012%
42	9.664	2676	2682	2691	rBV3	22392	42641	1.90%	0.193%
43	9.937	2759	2767	2781	rVB2	43130	67140	3.00%	0.304%
44	10.021	2783	2793	2813	rVB	270872	437766	19.54%	1.981%
45	10.220	2844	2855	2874	rBV	732940	1171798	52.30%	5.303%
46	10.522	2947	2949	2952	rBV4	1189	785	0.04%	0.004%
47	10.555	2957	2959	2965	rVB5	1007	755	0.03%	0.003%
48	10.587	2965	2969	2974	rBV5	1352	1456	0.06%	0.007%
49	10.673	2993	2996	2998	rBV4	1129	859	0.04%	0.004%
50	10.699	2998	3004	3006	rVV6	1202	1447	0.06%	0.007%
51	10.725	3008	3012	3016	rVB4	1779	1952	0.09%	0.009%
52	10.763	3021	3024	3027	rBV2	1845	1288	0.06%	0.006%
53	10.799	3027	3035	3042	rBV2	6789	11927	0.53%	0.054%
54	10.944	3073	3080	3089	rBV6	9110	12643	0.56%	0.057%
55	11.046	3104	3112	3127	rBV2	18617	31647	1.41%	0.143%
56	11.140	3139	3141	3145	rBV5	1662	945	0.04%	0.004%
57	11.185	3152	3155	3160	rVB5	1703	1079	0.05%	0.005%
58	11.255	3164	3177	3194	rBV	1173211	1798558	80.27%	8.140%
59	11.339	3201	3203	3206	rBV4	1590	903	0.04%	0.004%
60	11.419	3224	3228	3230	rBV5	2065	1388	0.06%	0.006%
61	11.432	3230	3232	3239	rVB4	1764	1105	0.05%	0.005%
62	11.493	3244	3251	3258	rBV4	9975	16755	0.75%	0.076%
63	11.538	3258	3265	3277	rVV4	18091	31796	1.42%	0.144%
64	11.632	3281	3294	3315	rVV	1170087	1833717	81.84%	8.299%
65	11.808	3346	3349	3352	rVB4	1768	946	0.04%	0.004%
66	11.886	3361	3373	3385	rBV3	35549	59683	2.66%	0.270%
67	11.989	3402	3405	3408	rVV5	1560	1015	0.05%	0.005%
68	12.104	3437	3441	3444	rBV4	1280	945	0.04%	0.004%
69	12.124	3444	3447	3451	rBV4	1111	998	0.04%	0.005%
70	12.243	3476	3484	3496	rVV6	12227	20535	0.92%	0.093%
71	12.291	3497	3499	3502	rBV3	1241	817	0.04%	0.004%
72	12.352	3512	3518	3519	rBV4	1686	1558	0.07%	0.007%
73	12.381	3521	3527	3539	rVV4	11445	18788	0.84%	0.085%
74	12.429	3540	3542	3547	rVB4	1408	1001	0.04%	0.005%
75	12.625	3597	3603	3606	rBV5	974	967	0.04%	0.004%
76	12.686	3620	3622	3625	rBV2	838	659	0.03%	0.003%

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Title : VOC Analysis

77	12.718	3628	3632	3635	rBV5	1008	731	0.03%	0.003%
78	12.747	3638	3641	3643	rBV4	1311	862	0.04%	0.004%
79	12.837	3657	3669	3684	rVV2	107555	167215	7.46%	0.757%
80	13.082	3744	3745	3751	rVB5	1413	782	0.03%	0.004%
81	13.149	3764	3766	3769	rBV2	896	656	0.03%	0.003%
82	13.165	3769	3771	3776	rVB5	805	687	0.03%	0.003%
83	13.342	3823	3826	3831	rVB5	1402	1303	0.06%	0.006%
84	13.439	3853	3856	3860	rBV3	1337	982	0.04%	0.004%
85	13.519	3874	3881	3883	rBV4	1786	1702	0.08%	0.008%
86	13.590	3899	3903	3906	rBV4	853	764	0.03%	0.003%
87	13.709	3936	3940	3941	rBV2	1130	742	0.03%	0.003%
88	13.779	3960	3962	3966	rVB3	1148	681	0.03%	0.003%
89	13.860	3984	3987	3991	rBV5	987	838	0.04%	0.004%
90	13.892	3994	3997	4002	rVB5	1237	956	0.04%	0.004%
91	14.088	4054	4058	4062	rBV5	1367	1342	0.06%	0.006%
92	14.609	4217	4220	4224	rBV6	1398	1144	0.05%	0.005%
93	14.628	4224	4226	4235	rVB8	1717	1505	0.07%	0.007%
94	14.722	4251	4255	4262	rVB4	1748	2081	0.09%	0.009%
95	14.757	4262	4266	4269	rBV6	1306	1166	0.05%	0.005%
96	14.959	4326	4329	4330	rBV2	1583	922	0.04%	0.004%
97	14.998	4339	4341	4343	rBV2	1709	664	0.03%	0.003%
98	15.307	4434	4437	4439	rBV3	1358	931	0.04%	0.004%
99	15.586	4521	4524	4526	rBV4	1381	1004	0.04%	0.005%
100	15.712	4561	4563	4567	rBV3	1355	819	0.04%	0.004%

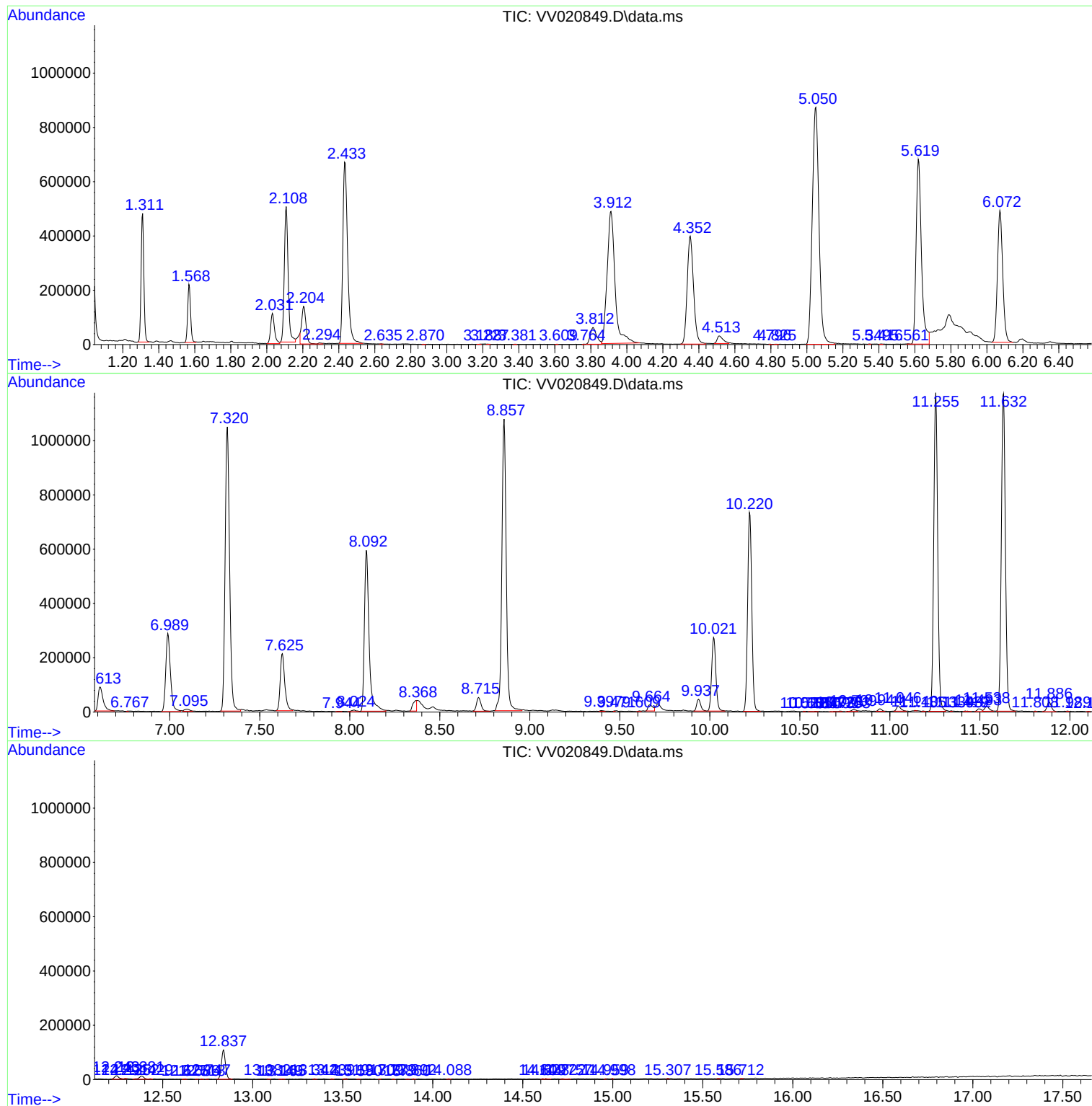
Sum of corrected areas: 22096275

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Instrument :
MSVOA_V
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040121\
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Instrument :
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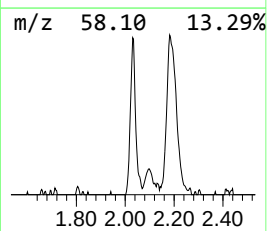
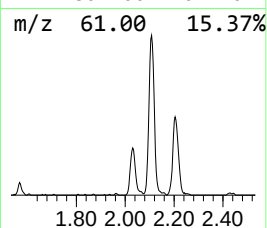
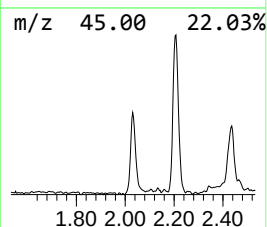
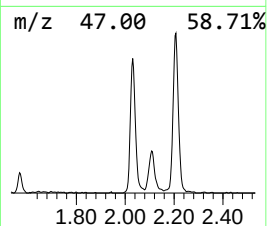
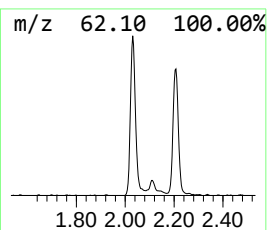
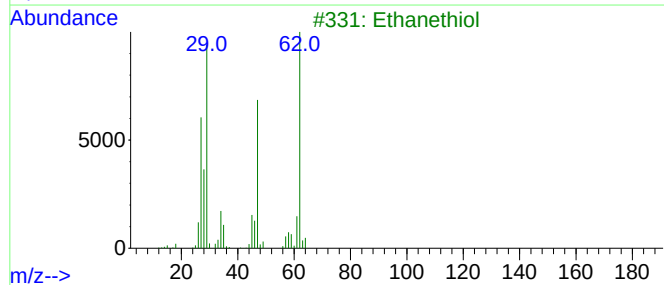
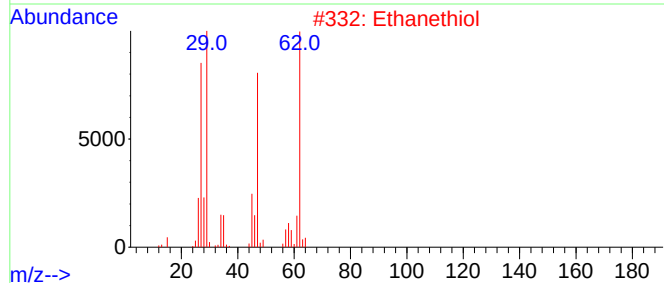
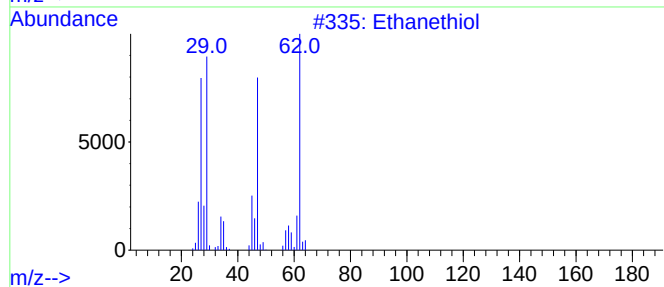
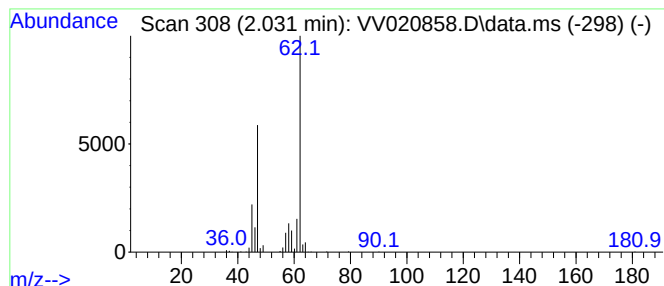
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.031	5.94 ug/L	168632	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol			62	C2H6S	000075-08-1	91
2	Ethanethiol			62	C2H6S	000075-08-1	91
3	Ethanethiol			62	C2H6S	000075-08-1	91
4	Ethanethiol			62	C2H6S	000075-08-1	91
5	Ethanethiol			62	C2H6S	000075-08-1	91



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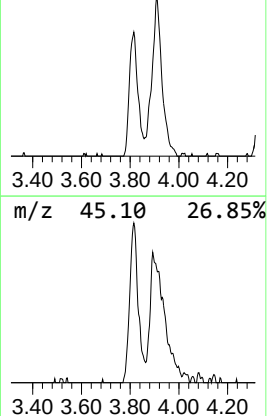
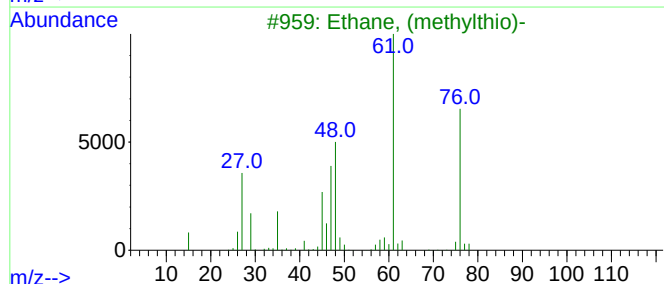
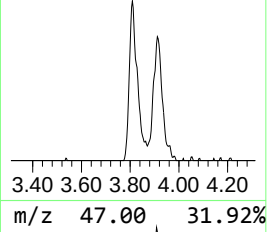
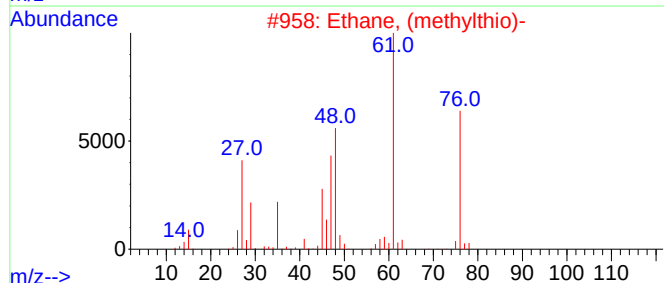
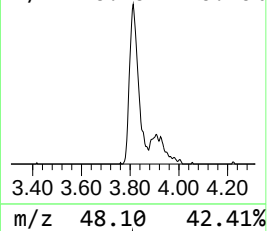
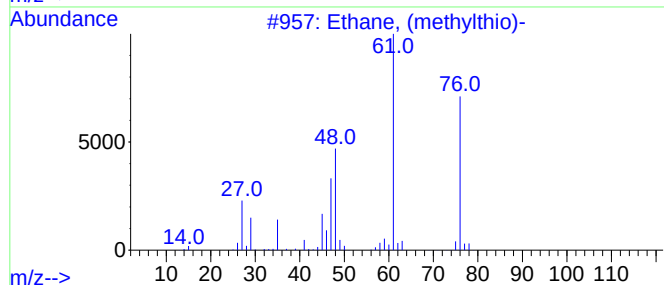
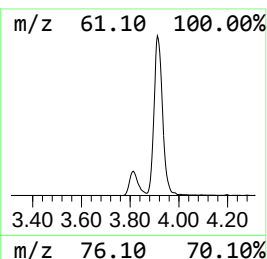
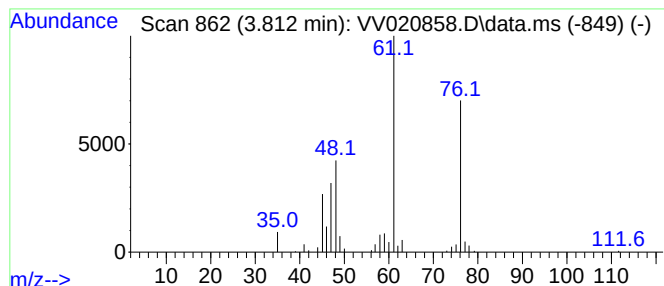
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethane, (methylthio)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.812	5.31 ug/L	150670	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, (methylthio)-	76	C3H8S	000624-89-5	94
2			Ethane, (methylthio)-	76	C3H8S	000624-89-5	94
3			Ethane, (methylthio)-	76	C3H8S	000624-89-5	94
4			Trimethylphosphine	76	C3H9P	000594-09-2	50
5			Propane, 1-(methylthio)-	90	C4H10S	003877-15-4	45



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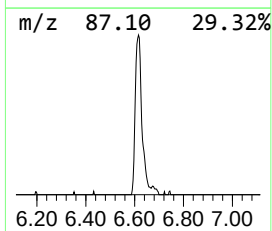
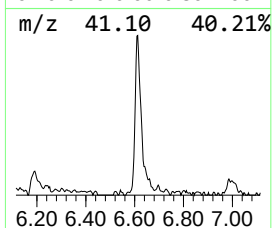
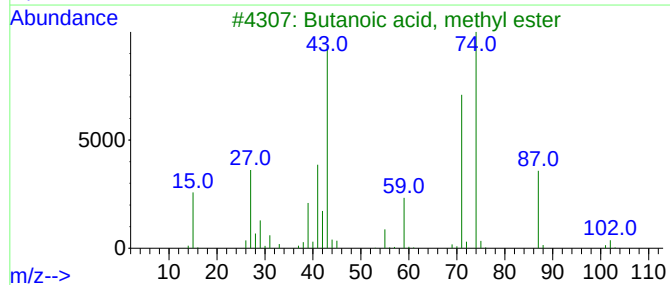
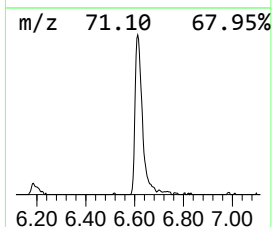
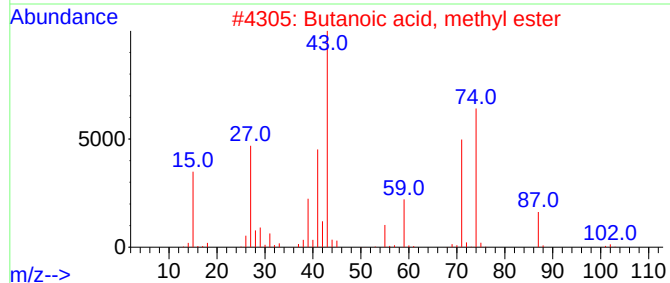
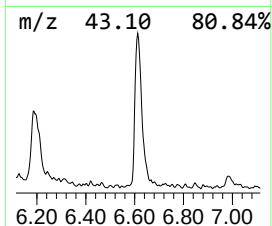
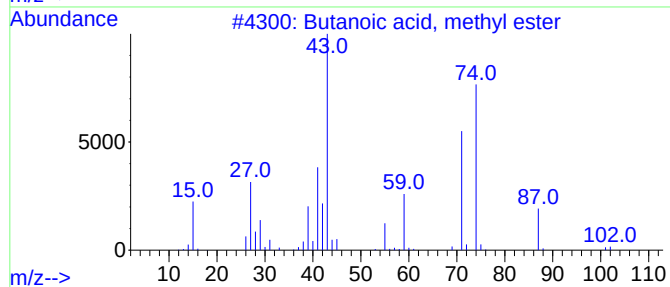
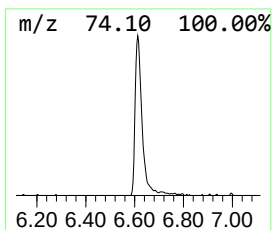
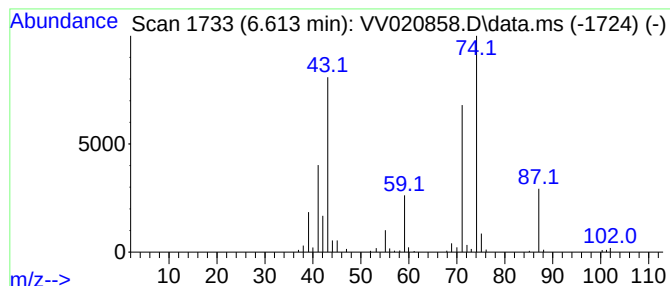
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.613	6.00 ug/L	170251	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
2			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	80
3			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	74
4			Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	42
5			Propanoic acid, 2-methyl-, methy...	102	C5H10O2	000547-63-7	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040121\
Data File : VV020858.D
Acq On : 01 Apr 2021 23:33
Operator : SY/MD
Sample : M1845-10
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW1B3

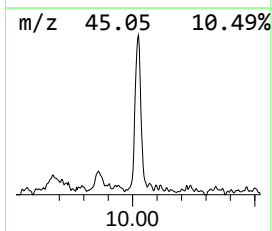
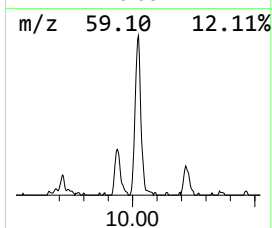
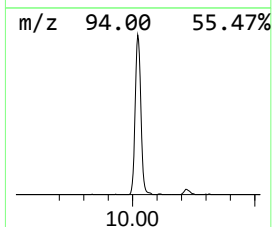
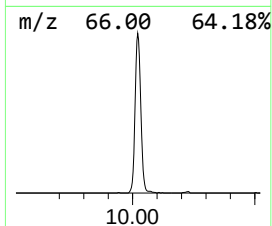
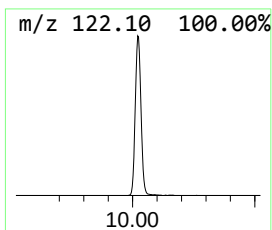
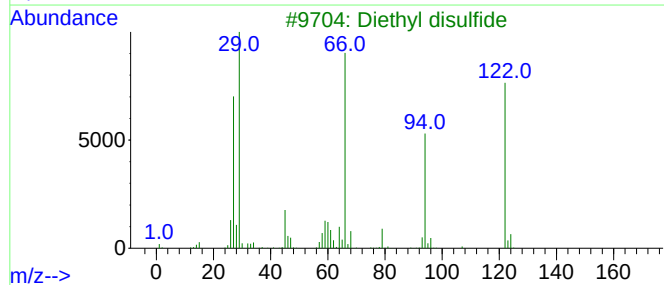
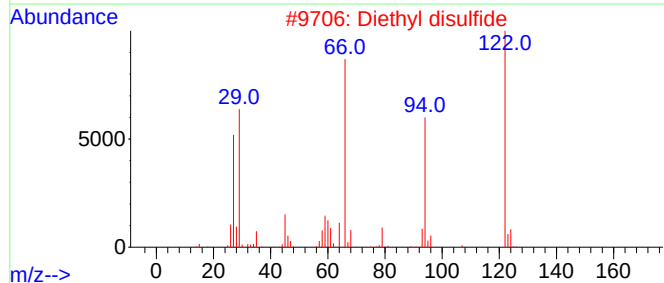
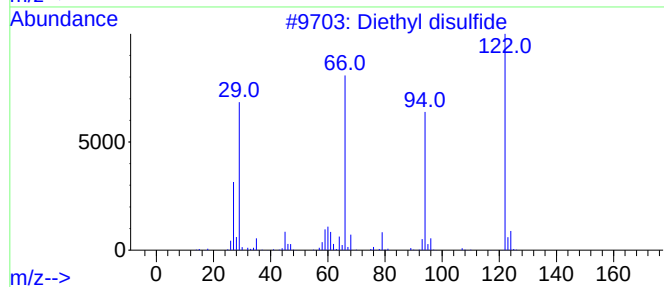
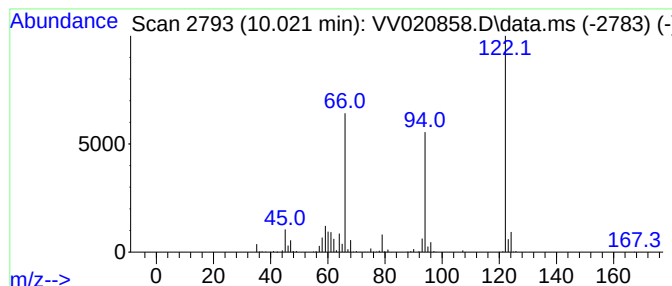
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Diethyl disulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.021	12.07 ug/L	437766	Chlorobenzene-d5	8.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyl disulfide	122	C4H10S2	000110-81-6	97
2			Diethyl disulfide	122	C4H10S2	000110-81-6	91
3			Diethyl disulfide	122	C4H10S2	000110-81-6	91
4			Benzene, ethoxy-	122	C8H10O	000103-73-1	42
5			Diethyl sulfone	122	C4H10O2S	000597-35-3	38



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Sample : M1845-10
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW1B3

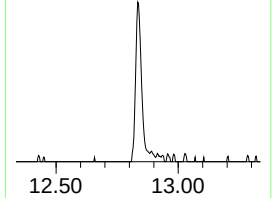
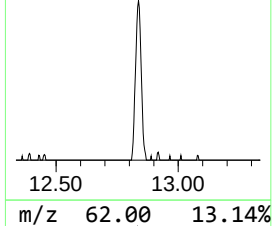
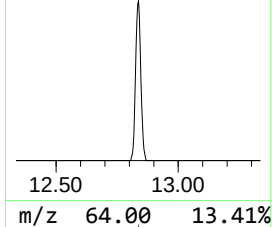
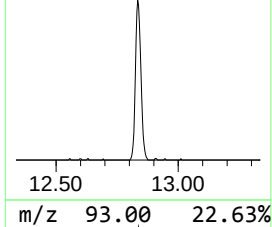
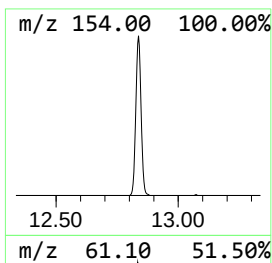
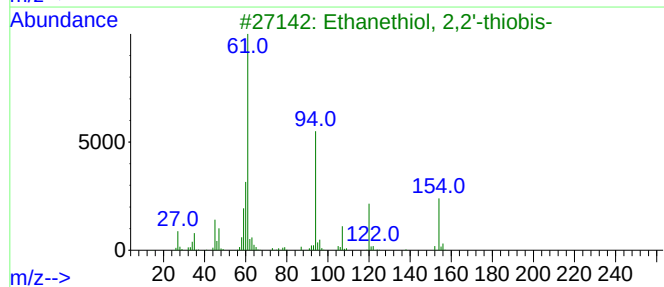
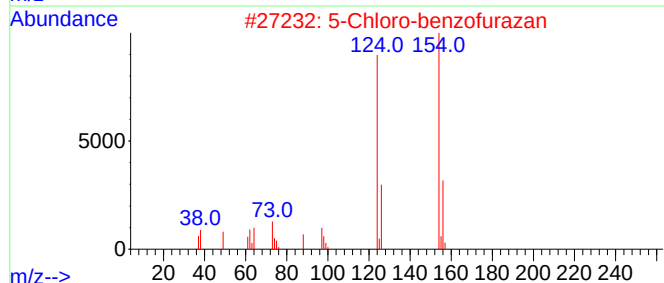
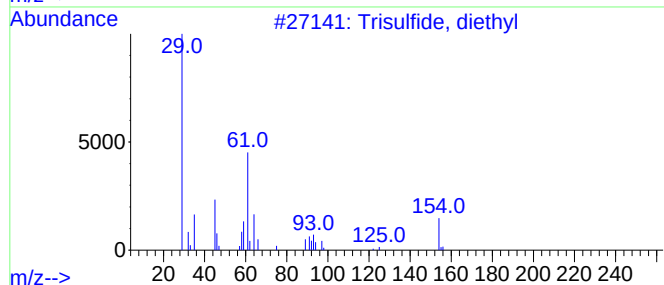
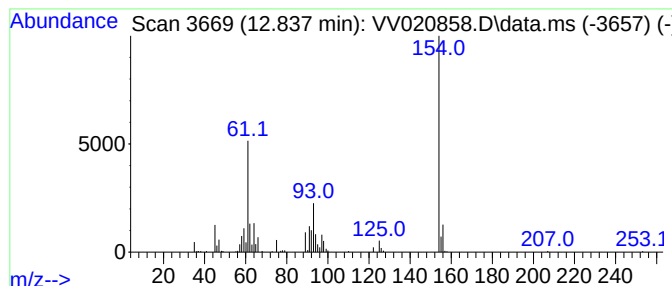
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trisulfide, diethyl Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.837	4.65 ug/L	167215	1,4-Dichlorobenzene-d4	11.255

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, diethyl	154	C4H10S3	003600-24-6	64
2			5-Chloro-benzofurazan	154	C6H3ClN2O	019155-86-3	46
3			Ethanethiol, 2,2'-thiobis-	154	C4H10S3	003570-55-6	28
4			1-Nitro-2-propanol	105	C3H7NO3	003156-73-8	22
5			1-Propanol, 3,3'-[1,2-ethanediyl...	210	C8H18O2S2	004756-21-2	22



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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW1B3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanethiol	2.031	5.9	ug/L	168632	1	5.622	1419910	50.0
Ethane, (methyl...	3.812	5.3	ug/L	150670	1	5.622	1419910	50.0
Butanoic acid, ...	6.613	6.0	ug/L	170251	1	5.622	1419910	50.0
Diethyl disulfide	10.021	12.1	ug/L	437766	2	8.857	1813120	50.0
Trisulfide, die...	12.837	4.7	ug/L	167215	3	11.255	1798560	50.0