

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060920\
 Data File : VV016704.D
 Acq On : 09 Jun 2020 10:06
 Operator : SY/MD
 Sample : L2875-01
 Misc : 5.0mL/MSVOA V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 ETTR8

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.315	63	70	80	rVB2	209299	231970	16.05%	2.045%
2	1.386	87	92	101	rVB	114755	122647	8.49%	1.081%
3	1.566	143	148	159	rVB	111505	125151	8.66%	1.103%
4	2.042	288	296	306	rBV	64091	93000	6.44%	0.820%
5	2.116	309	319	330	rVV	270387	435285	30.12%	3.837%
6	2.177	332	338	358	rVB	111111	182614	12.64%	1.610%
7	2.579	460	463	465	rBV4	907	521	0.04%	0.005%
8	2.592	465	467	468	rBV3	1134	425	0.03%	0.004%
9	2.637	479	481	482	rBV3	1089	405	0.03%	0.004%
10	2.753	514	517	519	rBV3	1533	1009	0.07%	0.009%
11	2.872	552	554	560	rVB7	1553	1080	0.07%	0.010%
12	2.897	560	562	563	rBV2	793	339	0.02%	0.003%
13	2.971	572	585	593	rBV7	8776	18315	1.27%	0.161%
14	3.048	607	609	612	rBV3	1121	528	0.04%	0.005%
15	3.119	629	631	633	rBV4	1210	454	0.03%	0.004%
16	3.158	641	643	644	rBV2	585	185	0.01%	0.002%
17	3.206	647	658	661	rBV2	3548	6010	0.42%	0.053%
18	3.257	672	674	681	rVB7	1860	1450	0.10%	0.013%
19	3.299	684	687	692	rBV7	943	946	0.07%	0.008%
20	3.338	696	699	702	rBV5	1248	831	0.06%	0.007%
21	3.357	702	705	707	rBV3	947	540	0.04%	0.005%
22	3.425	724	726	728	rBV3	1093	676	0.05%	0.006%
23	3.447	730	733	738	rVB4	1363	1312	0.09%	0.012%
24	3.515	752	754	755	rBV2	858	368	0.03%	0.003%
25	3.550	763	765	766	rBV2	1016	372	0.03%	0.003%
26	3.576	771	773	777	rVB3	979	435	0.03%	0.004%
27	3.611	783	784	786	rBV2	604	277	0.02%	0.002%
28	3.640	788	793	794	rVB4	944	570	0.04%	0.005%
29	3.656	794	798	800	rBV4	723	447	0.03%	0.004%
30	3.688	805	808	810	rBV3	1216	590	0.04%	0.005%
31	3.727	810	820	834	rBV4	17831	44548	3.08%	0.393%
32	3.897	863	873	891	rBV	132641	338475	23.42%	2.984%
33	4.717	1126	1128	1130	rVB4	884	330	0.02%	0.003%
34	4.820	1158	1160	1163	rBV3	999	671	0.05%	0.006%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
 Title : VOC Analysis

35	4.894	1181	1183	1185	rVB3	1124	512	0.04%	0.005%
36	4.913	1188	1189	1190	rBV	676	209	0.01%	0.002%
37	5.006	1216	1218	1219	rBV2	868	477	0.03%	0.004%
38	5.071	1221	1238	1260	rVV2	564598	1445100	100.00%	12.738%
39	5.479	1363	1365	1366	rBV2	843	371	0.03%	0.003%
40	5.640	1403	1415	1438	rBV	405358	796065	55.09%	7.017%
41	6.093	1544	1556	1581	rVB	327641	654008	45.26%	5.765%
42	6.203	1583	1590	1605	rVB2	20408	40159	2.78%	0.354%
43	6.524	1688	1690	1693	rBV4	1111	575	0.04%	0.005%
44	6.862	1793	1795	1796	rBV2	1052	322	0.02%	0.003%
45	6.926	1813	1815	1818	rVB4	826	347	0.02%	0.003%
46	7.006	1830	1840	1859	rBV	197073	341718	23.65%	3.012%
47	7.338	1932	1943	1958	rBV	668862	1131026	78.27%	9.970%
48	7.640	2029	2037	2055	rVB	138572	229393	15.87%	2.022%
49	7.862	2103	2106	2109	rBV4	1779	1274	0.09%	0.011%
50	8.109	2172	2183	2221	rBV	466454	877324	60.71%	7.733%
51	8.527	2311	2313	2318	rVB5	1461	1025	0.07%	0.009%
52	8.736	2369	2378	2390	rVB4	20144	34938	2.42%	0.308%
53	8.874	2410	2421	2446	rVB	608124	987620	68.34%	8.706%
54	9.421	2589	2591	2593	rBV3	1342	699	0.05%	0.006%
55	9.501	2611	2616	2617	rBV4	1988	1478	0.10%	0.013%
56	9.563	2631	2635	2636	rBV5	1963	1228	0.08%	0.011%
57	9.717	2681	2683	2684	rBV2	1930	737	0.05%	0.006%
58	10.038	2771	2783	2796	rBV	197251	312474	21.62%	2.754%
59	10.238	2831	2845	2866	rBV	468824	743754	51.47%	6.556%
60	10.604	2954	2959	2964	rBV3	5917	7431	0.51%	0.066%
61	10.775	3008	3012	3014	rBV4	1876	1532	0.11%	0.014%
62	11.032	3090	3092	3093	rBV2	1264	518	0.04%	0.005%
63	11.054	3096	3099	3100	rBV3	1283	654	0.05%	0.006%
64	11.132	3120	3123	3129	rBV9	2270	3059	0.21%	0.027%
65	11.270	3156	3166	3186	rVB	631198	961582	66.54%	8.476%
66	11.556	3249	3255	3264	rBV4	9618	15524	1.07%	0.137%
67	11.646	3273	3283	3306	rVB	710899	1122491	77.68%	9.895%
68	12.485	3542	3544	3547	rBV4	1150	595	0.04%	0.005%
69	13.054	3717	3721	3726	rBV7	1643	1665	0.12%	0.015%
70	13.128	3742	3744	3750	rVB6	1362	1377	0.10%	0.012%
71	13.154	3750	3752	3754	rBV4	1415	645	0.04%	0.006%

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 Title : VOC Analysis

72	13.540	3870	3872	3875	rVB4	2707	970	0.07%	0.009%
73	13.585	3883	3886	3891	rVB6	1929	1962	0.14%	0.017%
74	13.607	3891	3893	3896	rBV4	1616	1042	0.07%	0.009%
75	13.820	3958	3959	3960	rBV	903	279	0.02%	0.002%
76	14.607	4202	4204	4207	rBV3	1383	779	0.05%	0.007%
77	14.746	4246	4247	4249	rBV2	1044	358	0.02%	0.003%
78	14.758	4249	4251	4255	rBV6	1536	1307	0.09%	0.012%
79	15.003	4325	4327	4330	rBV3	1300	914	0.06%	0.008%
80	15.238	4396	4400	4403	rBV6	1627	1423	0.10%	0.013%
81	15.607	4513	4515	4521	rVB6	1837	1232	0.09%	0.011%
82	15.636	4521	4524	4527	rBV5	2168	1636	0.11%	0.014%

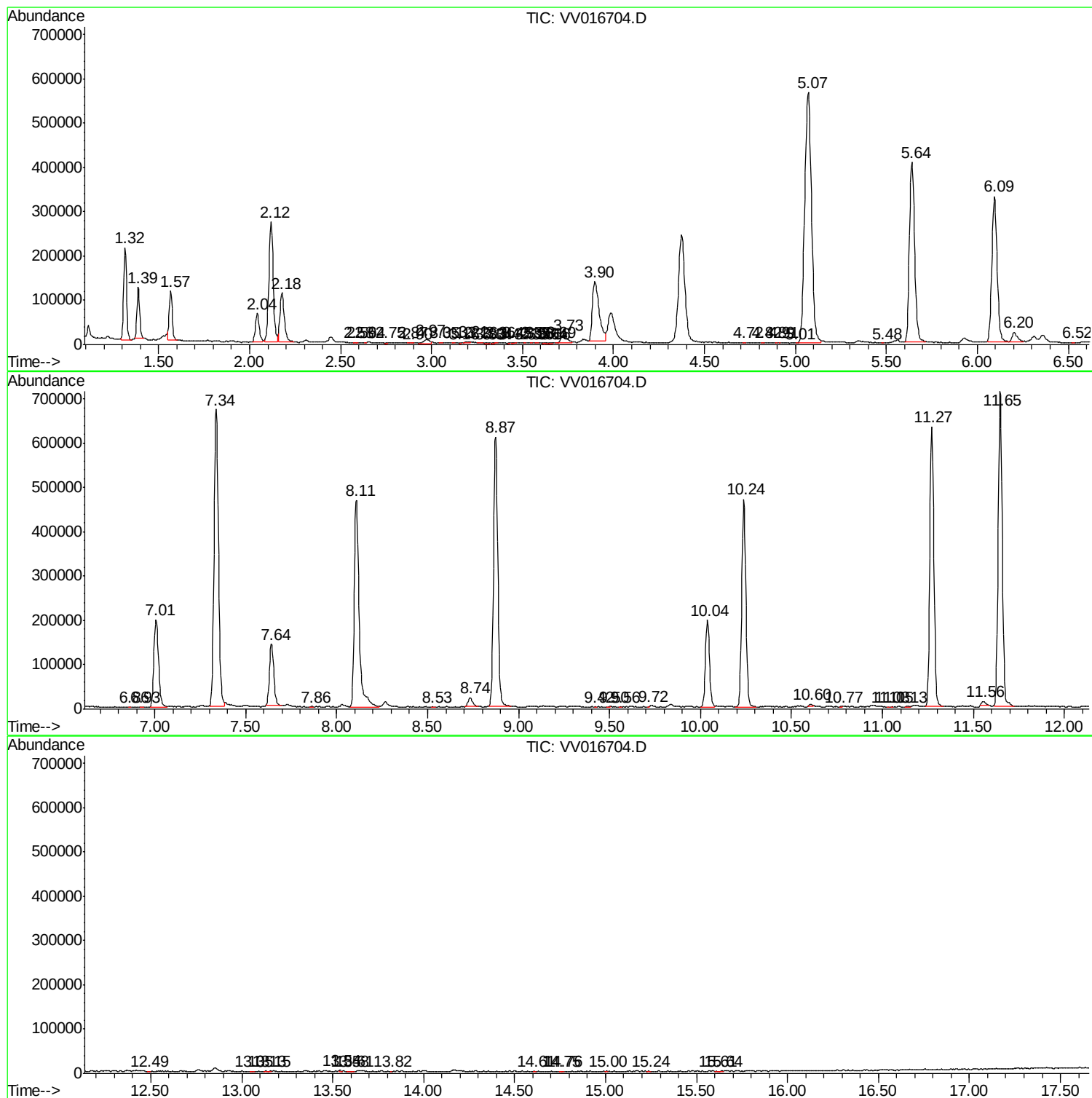
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060920\
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
ETTR8

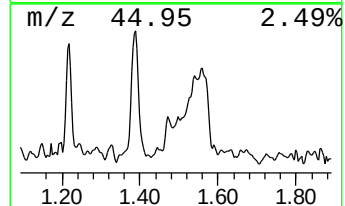
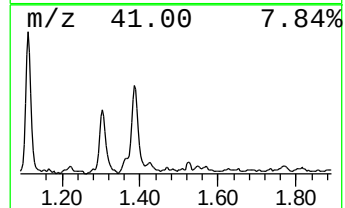
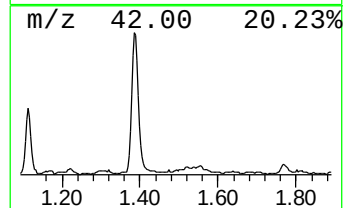
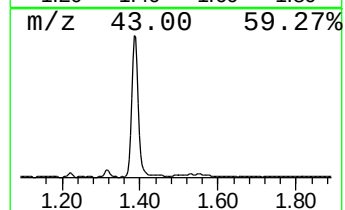
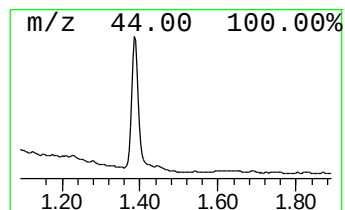
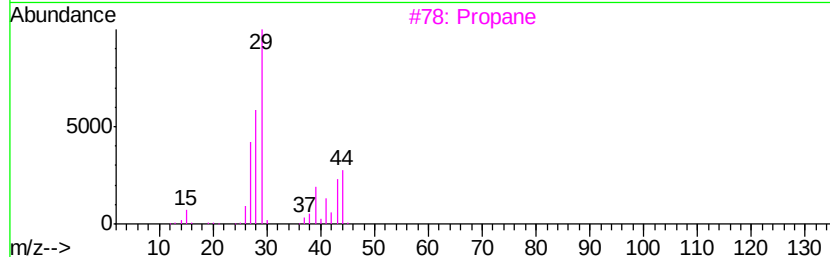
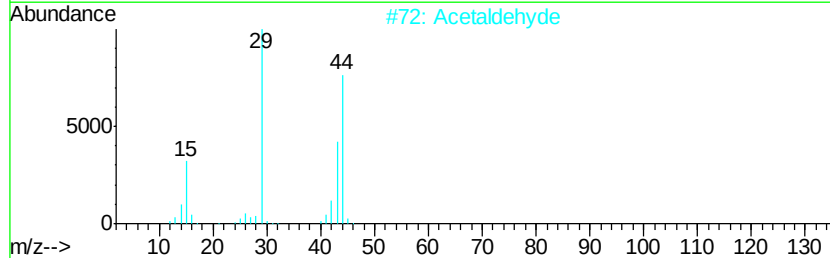
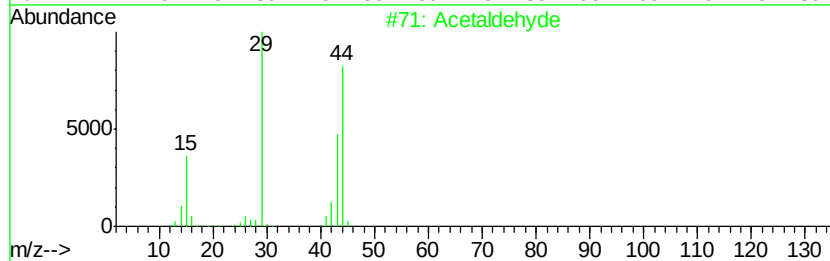
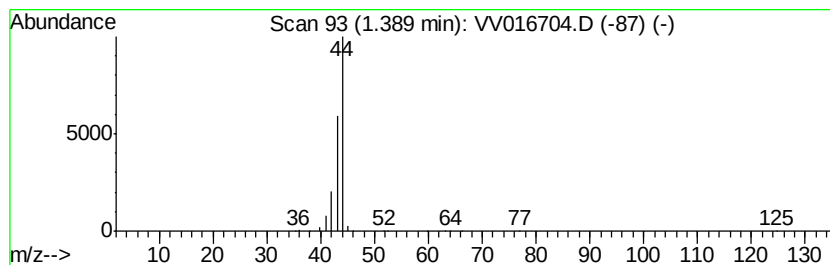
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.39	7.70 ug/L	122647	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetaldehyde	44	C2H4O	000075-07-0	9
2		Acetaldehyde	44	C2H4O	000075-07-0	9
3		Propane	44	C3H8	000074-98-6	5
4		Ethylene oxide	44	C2H4O	000075-21-8	5
5		Ethylene oxide	44	C2H4O	000075-21-8	5



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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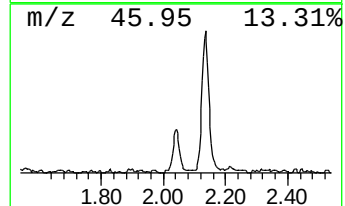
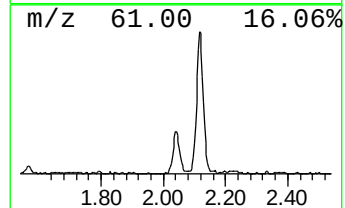
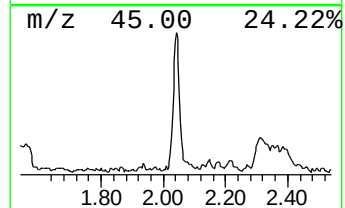
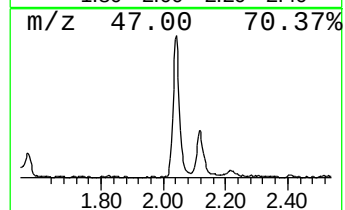
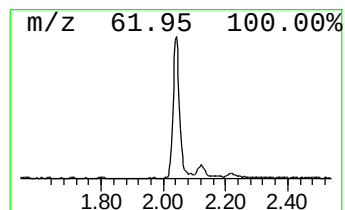
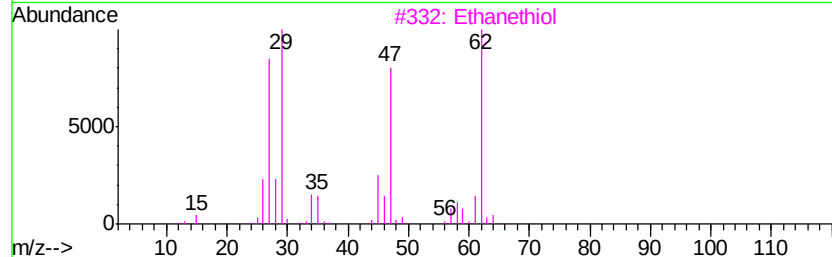
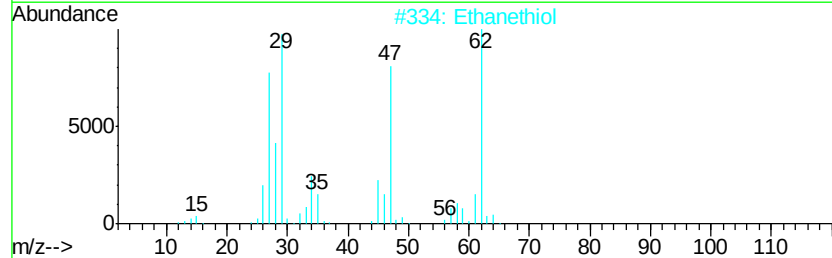
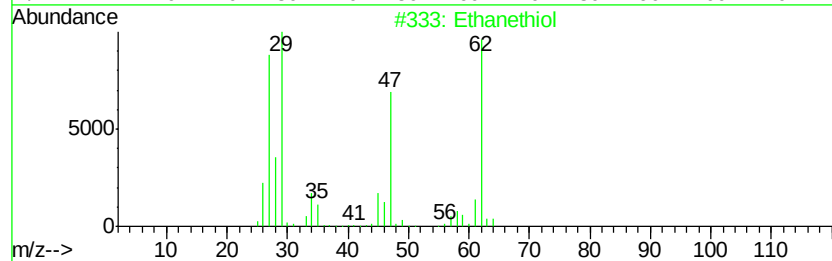
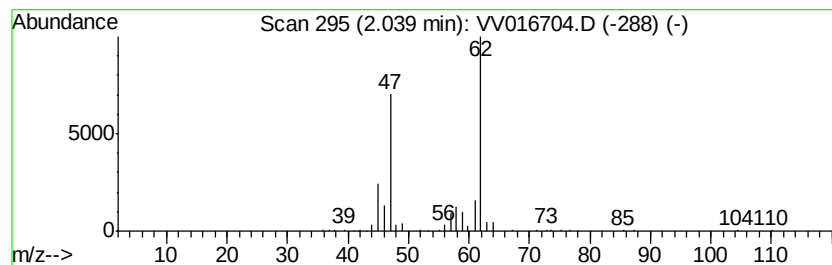
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Ethanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.04	5.84 ug/L	93000	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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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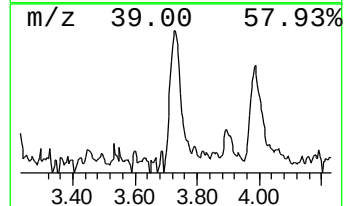
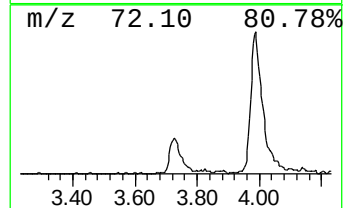
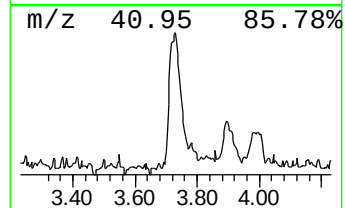
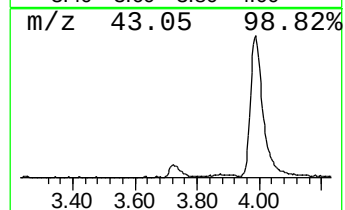
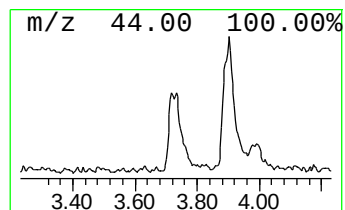
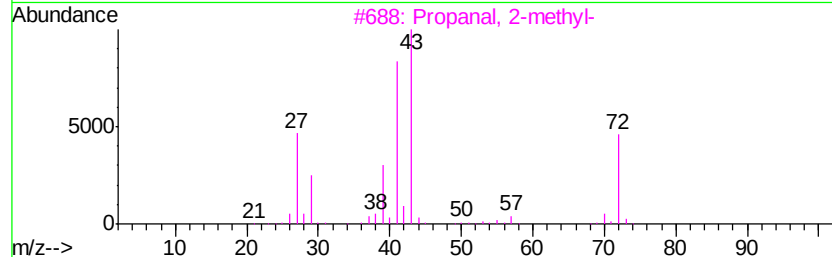
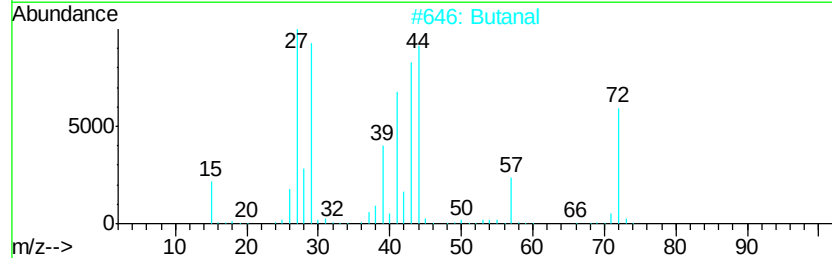
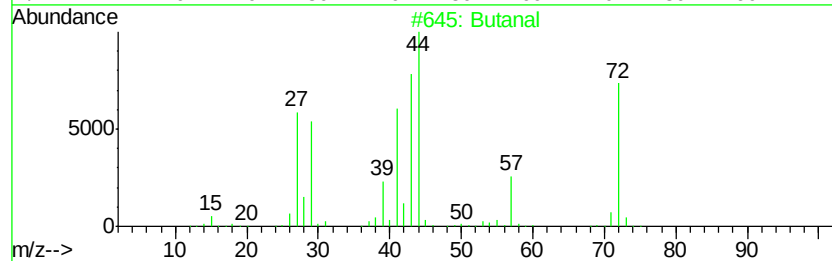
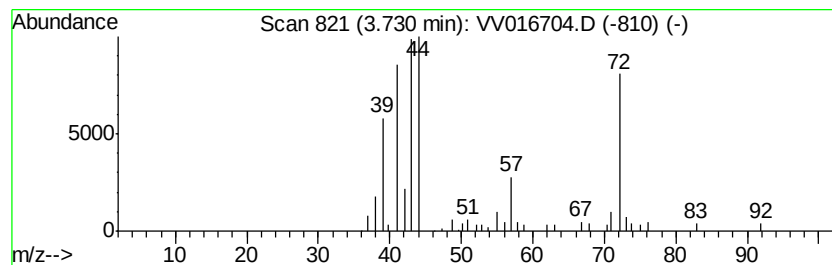
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.73	2.80 ug/L	44548	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	58
2		Butanal	72	C4H8O	000123-72-8	53
3		Propanal, 2-methyl-	72	C4H8O	000078-84-2	47
4		Butanal	72	C4H8O	000123-72-8	47
5		Butanal, 3-methyl-	86	C5H10O	000590-86-3	37



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Instrument :
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ClientSampled :
ETTR8

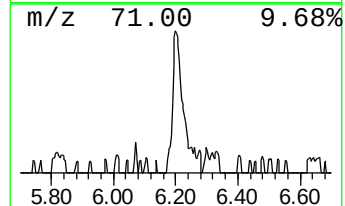
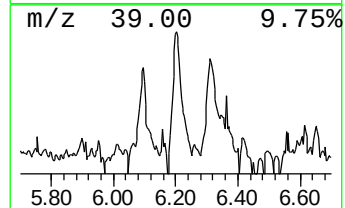
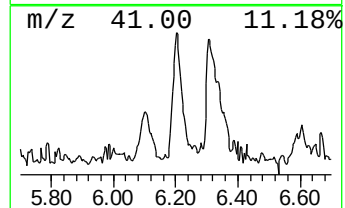
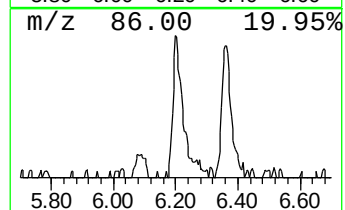
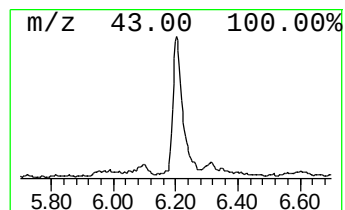
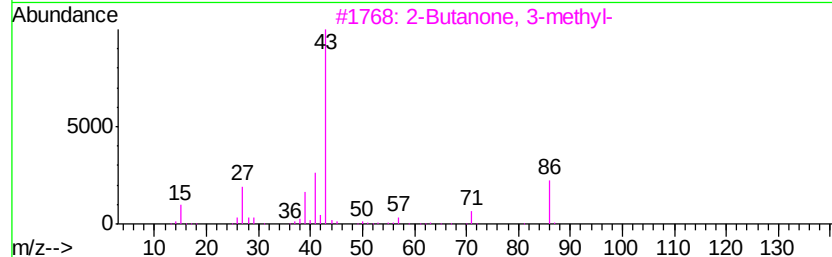
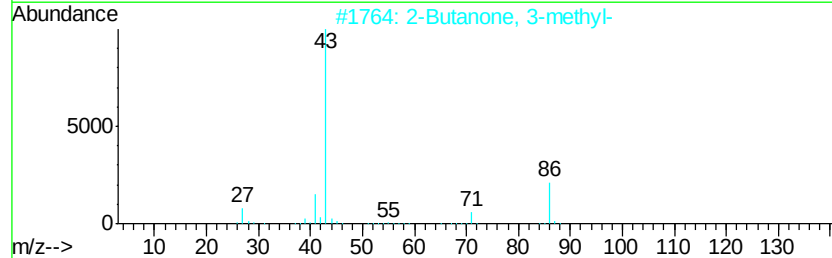
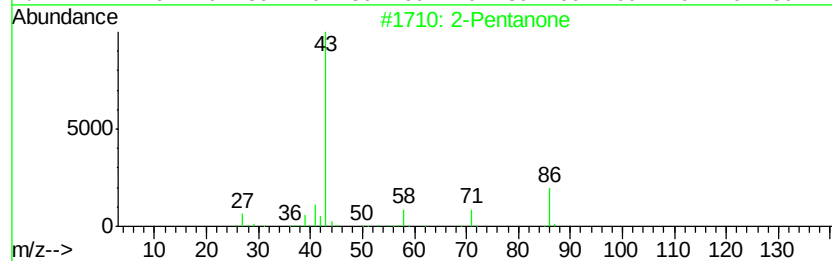
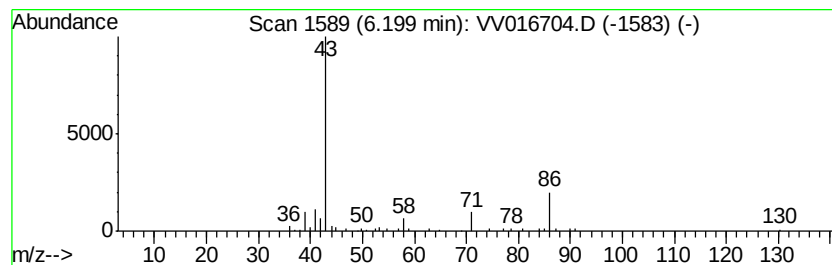
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Quant Title : VOC Analysis

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

Peak Number 4 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.20	2.52 ug/L	40159	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone	86	C5H10O	000107-87-9	72
2		2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53
3		2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53
4		2-Pentanone	86	C5H10O	000107-87-9	47
5		2-Pentanone	86	C5H10O	000107-87-9	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060920\
Data File : VV016704.D
Acq On : 09 Jun 2020 10:06
Operator : SY/MD
Sample : L2875-01
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
ETTR8

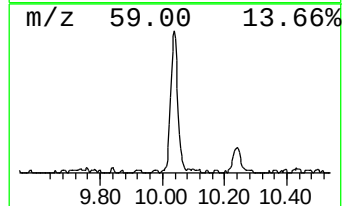
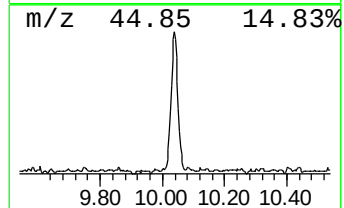
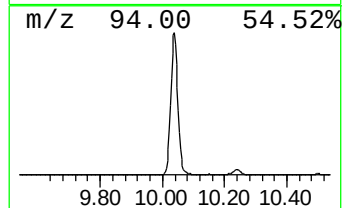
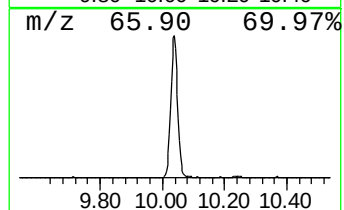
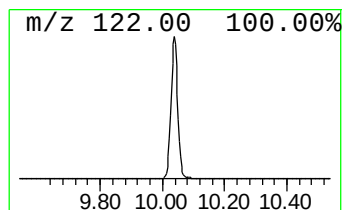
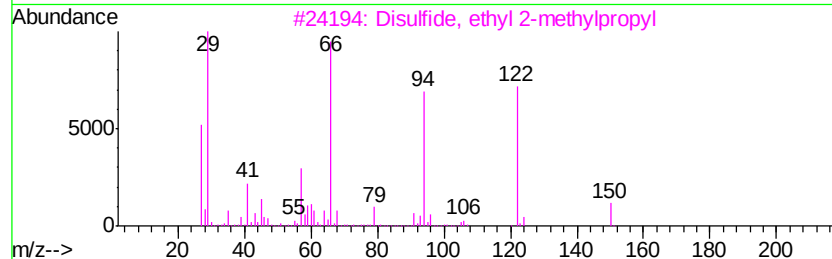
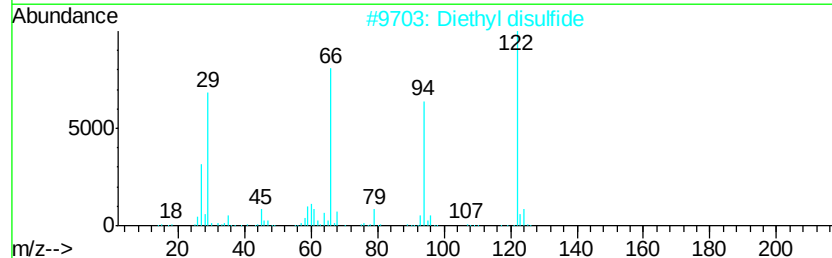
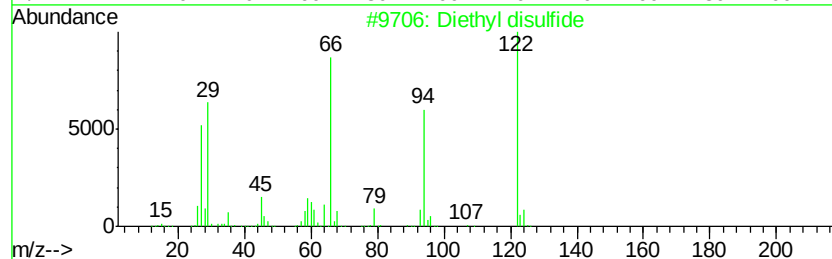
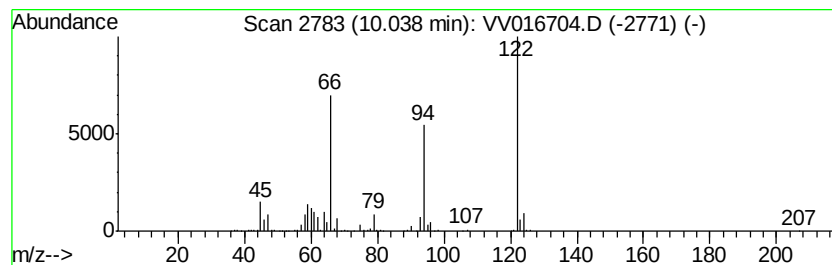
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Diethyl disulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.04	15.82 ug/L	312474	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethyl disulfide	122	C4H10S2	000110-81-6	95
2		Diethyl disulfide	122	C4H10S2	000110-81-6	91
3		Disulfide, ethyl 2-methylpropyl	150	C6H14S2	040136-66-1	64
4		Diethyl disulfide	122	C4H10S2	000110-81-6	45
5		Benzene, ethoxy-	122	C8H10O	000103-73-1	45



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060920\
Data File : VV016704.D
Acq On : 09 Jun 2020 10:06
Operator : SY/MD
Sample : L2875-01
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
ETTR8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.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
unknown-01	1.39	7.7	ug/L	122647	1	5.64	796065	50.0
Ethanethiol	2.04	5.8	ug/L	93000	1	5.64	796065	50.0
Butanal	3.73	2.8	ug/L	44548	1	5.64	796065	50.0
2-Pentanone	6.20	2.5	ug/L	40159	1	5.64	796065	50.0
Diethyl disulfide	10.04	15.8	ug/L	312474	2	8.87	987620	50.0