

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
 Data File : VV029716.D
 Acq On : 19 Dec 2022 13:05
 Operator : SY/MD
 Sample : N6075-06 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGSM0

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\SFAMVLM120722WMA.M
 Title : VOC Analysis

Signal : TIC: VV029716.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	76	82	96	rVB	213516	213453	14.62%	1.693%
2	1.565	156	163	176	rVB	173397	192044	13.15%	1.523%
3	2.105	321	331	343	rBV	350690	498247	34.12%	3.952%
4	2.465	439	443	445	rBV2	300	211	0.01%	0.002%
5	2.503	445	455	472	rVB	10173	16429	1.13%	0.130%
6	2.732	521	526	531	rBV3	425	503	0.03%	0.004%
7	2.780	539	541	544	rBV2	174	100	0.01%	0.001%
8	2.819	549	553	555	rBV2	171	145	0.01%	0.001%
9	2.992	603	607	614	rVB2	177	201	0.01%	0.002%
10	3.031	614	619	621	rBV	231	167	0.01%	0.001%
11	3.053	623	626	630	rVB	240	148	0.01%	0.001%
12	3.101	634	641	643	rBV	202	213	0.01%	0.002%
13	3.179	659	665	667	rBV2	512	575	0.04%	0.005%
14	3.327	708	711	714	rVB	137	84	0.01%	0.001%
15	3.381	725	728	733	rVB2	247	199	0.01%	0.002%
16	3.410	733	737	740	rBV2	130	108	0.01%	0.001%
17	3.455	748	751	753	rBV	149	106	0.01%	0.001%
18	3.587	786	792	797	rBV	175	209	0.01%	0.002%
19	3.622	801	803	808	rVB	145	97	0.01%	0.001%
20	3.648	808	811	813	rBV2	160	104	0.01%	0.001%
21	3.706	824	829	834	rBV2	180	265	0.02%	0.002%
22	3.790	851	855	859	rBV2	200	185	0.01%	0.001%
23	3.876	871	882	920	rBV2	94508	288829	19.78%	2.291%
24	4.339	1009	1026	1066	rBV	227216	564248	38.64%	4.476%
25	4.597	1103	1106	1110	rBV2	325	185	0.01%	0.001%
26	4.632	1114	1117	1118	rBV2	226	107	0.01%	0.001%
27	4.674	1128	1130	1132	rBV	232	86	0.01%	0.001%
28	4.712	1139	1142	1146	rVB3	181	110	0.01%	0.001%
29	4.745	1146	1152	1154	rVB3	310	152	0.01%	0.001%
30	4.802	1166	1170	1174	rBV2	106	94	0.01%	0.001%
31	4.825	1174	1177	1178	rBV	292	160	0.01%	0.001%
32	4.970	1220	1222	1226	rVB	198	82	0.01%	0.001%
33	5.040	1226	1244	1295	rBV2	554947	1460215	100.00%	11.583%
34	5.281	1309	1319	1335	rBV2	10719	26833	1.84%	0.213%
35	5.510	1389	1390	1395	rBV	124	85	0.01%	0.001%
36	5.548	1400	1402	1404	rBV3	191	127	0.01%	0.001%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
 Title : VOC Analysis

37	5.609	1408	1421	1452	rBV	511094	1039724	71.20%	8.247%
38	5.905	1504	1513	1525	rVB4	4725	9993	0.68%	0.079%
39	6.063	1547	1562	1600	rBV	310918	654479	44.82%	5.191%
40	6.240	1615	1617	1619	rBV2	356	198	0.01%	0.002%
41	6.275	1625	1628	1632	rVB2	501	399	0.03%	0.003%
42	6.297	1632	1635	1639	rBV3	569	474	0.03%	0.004%
43	6.355	1643	1653	1658	rBV	4669	8936	0.61%	0.071%
44	6.461	1676	1686	1721	rBV	131296	262666	17.99%	2.083%
45	6.828	1798	1800	1804	rVB2	304	181	0.01%	0.001%
46	6.924	1826	1830	1834	rBV2	179	165	0.01%	0.001%
47	6.979	1834	1847	1885	rVV	158768	297747	20.39%	2.362%
48	7.182	1899	1910	1921	rBV	31151	55745	3.82%	0.442%
49	7.307	1937	1949	1983	rBV	685799	1218587	83.45%	9.666%
50	7.613	2033	2044	2075	rBV2	145538	263550	18.05%	2.091%
51	7.854	2117	2119	2121	rBV2	428	198	0.01%	0.002%
52	7.918	2129	2139	2156	rBV	41002	69977	4.79%	0.555%
53	8.082	2181	2190	2214	rBV	336312	611496	41.88%	4.850%
54	8.188	2216	2223	2243	rVB	71224	119763	8.20%	0.950%
55	8.301	2250	2258	2272	rVB	37744	61958	4.24%	0.491%
56	8.458	2303	2307	2310	rBV3	479	441	0.03%	0.003%
57	8.532	2327	2330	2331	rBV3	223	126	0.01%	0.001%
58	8.542	2331	2333	2336	rVV2	222	128	0.01%	0.001%
59	8.593	2347	2349	2350	rBV	280	124	0.01%	0.001%
60	8.613	2353	2355	2360	rVB2	755	613	0.04%	0.005%
61	8.674	2363	2374	2400	rBV	122631	201504	13.80%	1.598%
62	8.844	2415	2427	2451	rBV	768725	1261580	86.40%	10.007%
63	9.211	2537	2541	2544	rVB2	212	155	0.01%	0.001%
64	9.239	2548	2550	2554	rBV	213	133	0.01%	0.001%
65	9.307	2568	2571	2573	rBV	122	86	0.01%	0.001%
66	9.330	2576	2578	2580	rVV	150	80	0.01%	0.001%
67	9.384	2589	2595	2606	rVB3	1430	2387	0.16%	0.019%
68	9.432	2606	2610	2613	rBV2	275	215	0.01%	0.002%
69	9.477	2622	2624	2629	rVB2	204	103	0.01%	0.001%
70	9.506	2629	2633	2634	rBV	240	166	0.01%	0.001%
71	9.542	2636	2644	2658	rVB	10367	15930	1.09%	0.126%
72	9.600	2658	2662	2667	rBV3	237	270	0.02%	0.002%
73	9.667	2680	2683	2686	rBV	341	186	0.01%	0.001%
74	9.728	2698	2702	2704	rBV3	224	175	0.01%	0.001%
75	10.024	2792	2794	2800	rBV2	258	153	0.01%	0.001%
76	10.088	2812	2814	2817	rVB	196	87	0.01%	0.001%

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Title : VOC Analysis

77	10.162	2828	2837	2841	rBV	17607	25738	1.76%	0.204%
78	10.207	2842	2851	2873	rVB	442446	698549	47.84%	5.541%
79	10.336	2889	2891	2893	rBV	210	94	0.01%	0.001%
80	10.374	2896	2903	2911	rVB4	1371	2192	0.15%	0.017%
81	10.477	2928	2935	2938	rBV2	193	243	0.02%	0.002%
82	10.493	2938	2940	2942	rBV	195	113	0.01%	0.001%
83	10.542	2953	2955	2956	rBV	358	182	0.01%	0.001%
84	10.567	2956	2963	2978	rVB2	8457	13922	0.95%	0.110%
85	10.625	2978	2981	2984	rBV	218	137	0.01%	0.001%
86	10.725	3009	3012	3016	rVB2	270	172	0.01%	0.001%
87	10.818	3038	3041	3043	rBV	156	99	0.01%	0.001%
88	10.844	3045	3049	3050	rBV3	359	207	0.01%	0.002%
89	10.905	3065	3068	3071	rBV	522	428	0.03%	0.003%
90	10.973	3085	3089	3092	rBV2	180	179	0.01%	0.001%
91	11.114	3130	3133	3136	rBV2	217	125	0.01%	0.001%
92	11.175	3147	3152	3159	rBV4	724	999	0.07%	0.008%
93	11.236	3159	3171	3198	rBV	831215	1297719	88.87%	10.294%
94	11.522	3258	3260	3267	rVB	318	196	0.01%	0.002%
95	11.561	3267	3272	3275	rBV3	340	356	0.02%	0.003%
96	11.612	3275	3288	3311	rBV	725303	1137275	77.88%	9.021%
97	11.764	3333	3335	3337	rBV2	470	200	0.01%	0.002%
98	12.040	3417	3421	3428	rBV3	386	674	0.05%	0.005%
99	12.362	3518	3521	3523	rBV2	280	188	0.01%	0.001%
100	13.252	3793	3798	3804	rBV4	936	1017	0.07%	0.008%

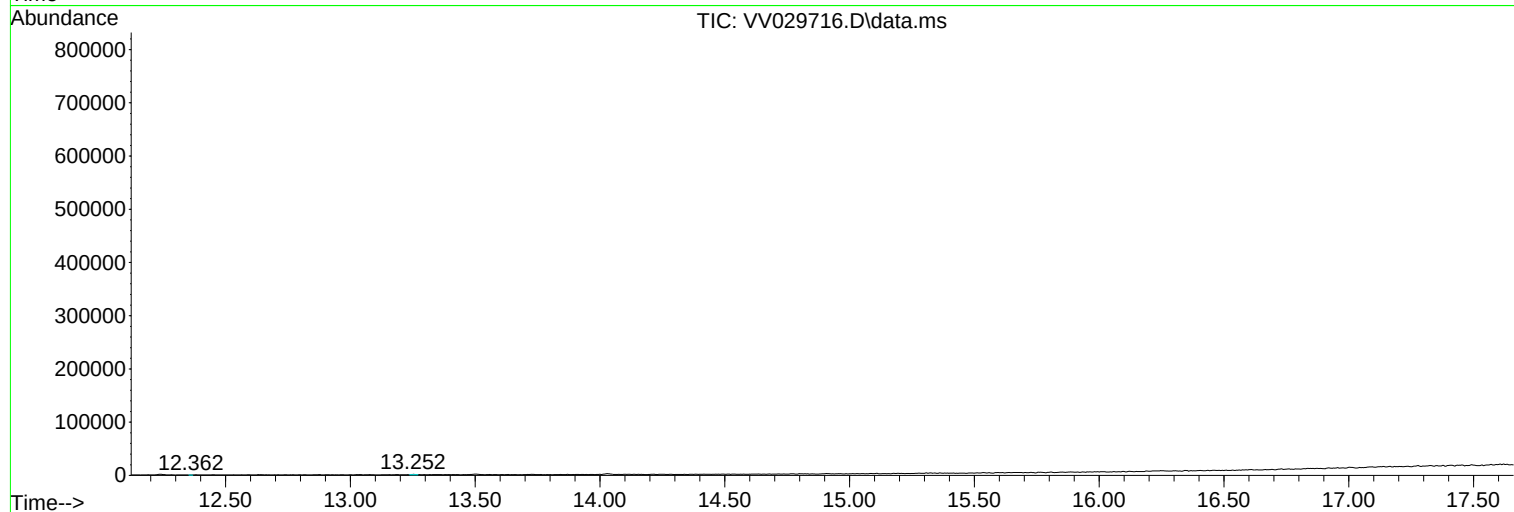
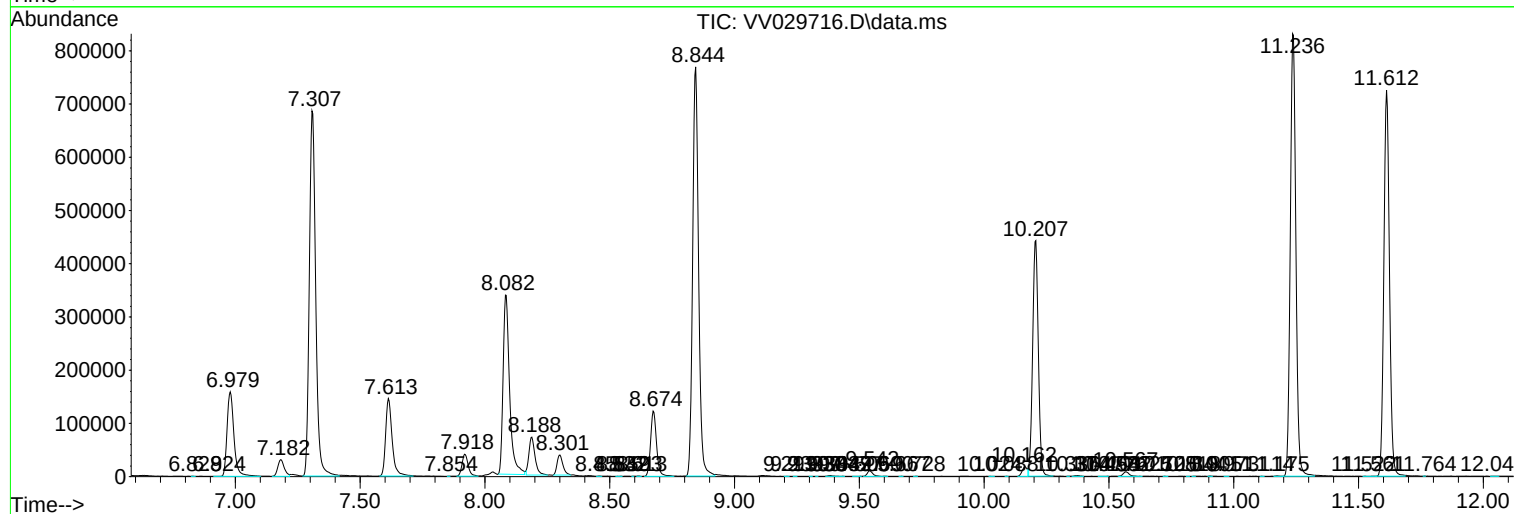
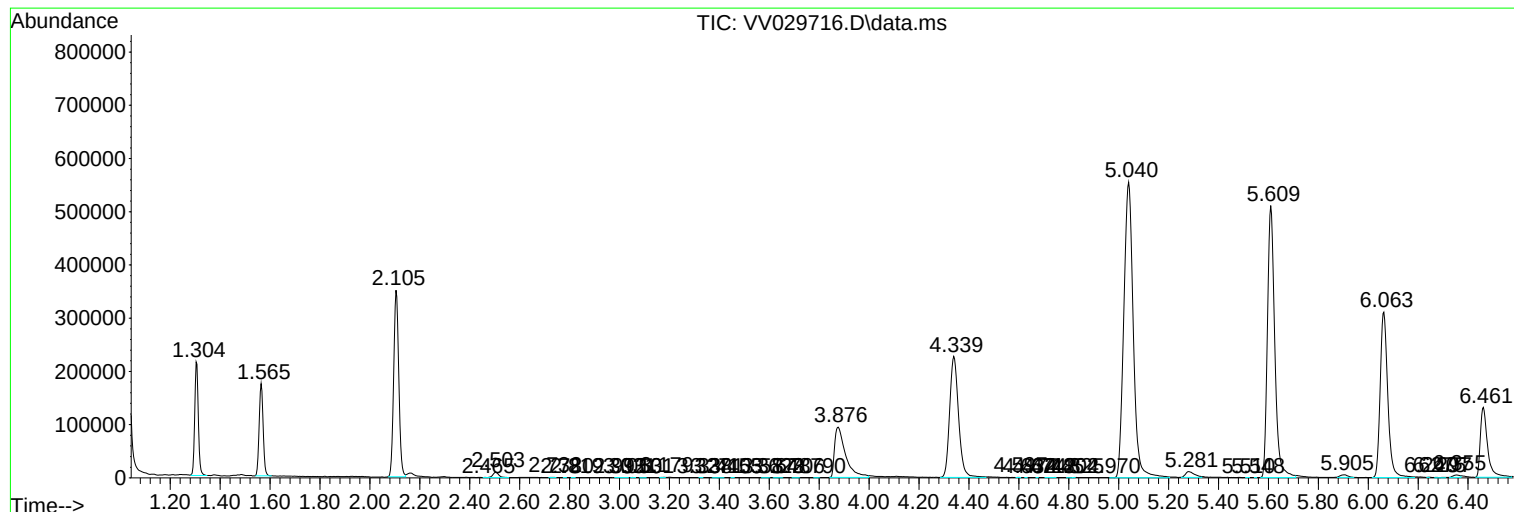
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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



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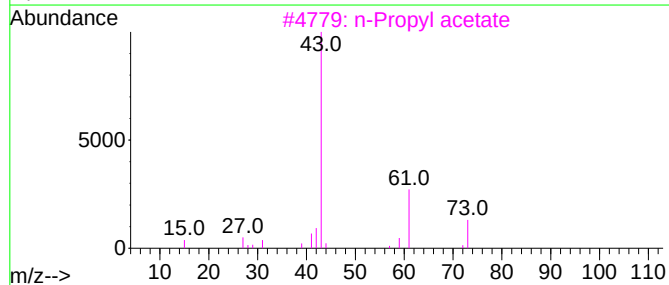
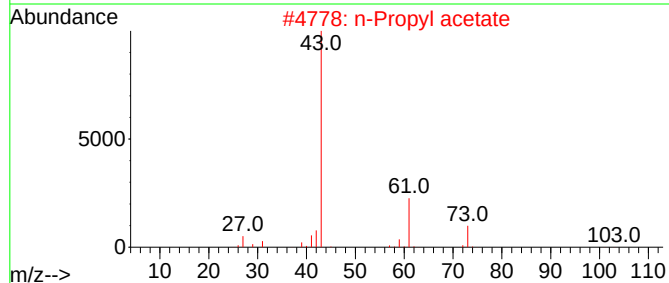
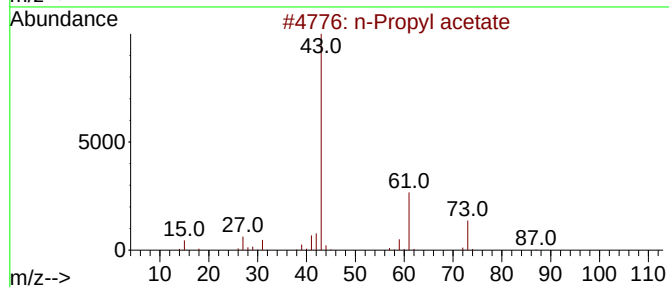
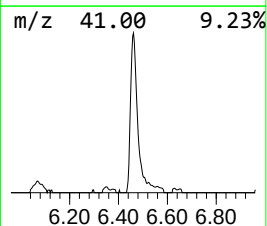
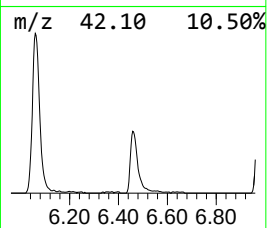
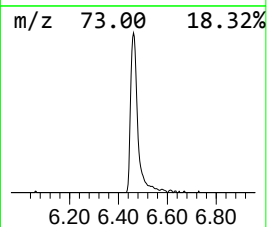
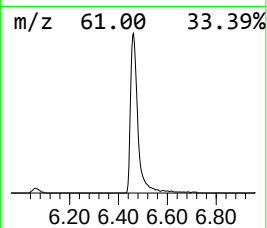
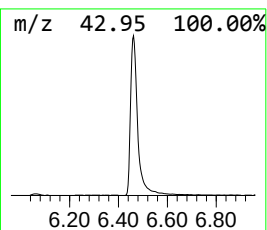
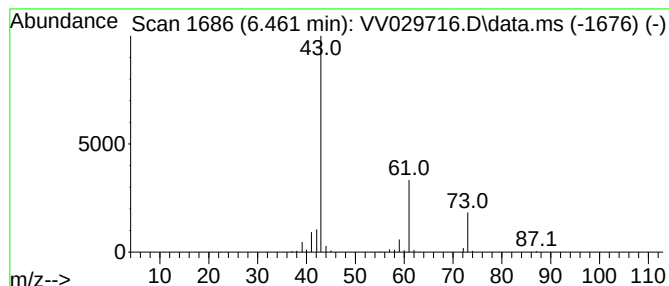
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.461	12.63 ug/L	262666	1,4-Difluorobenzene	5.609

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	83
2	n-Propyl acetate			102	C5H10O2	000109-60-4	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	Propanal, 2,3-dihydroxy-, (S)-			90	C3H6O3	000497-09-6	36



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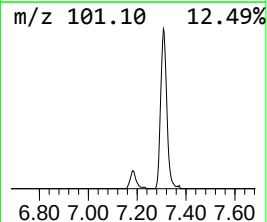
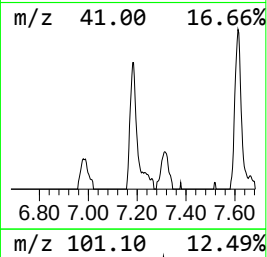
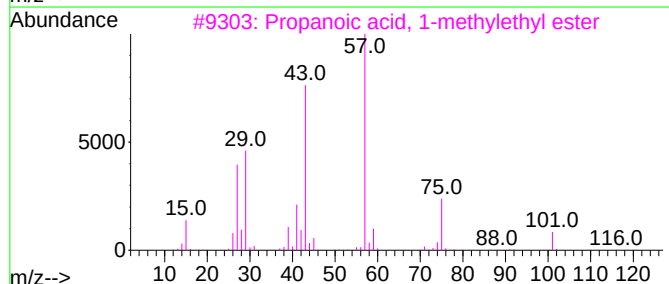
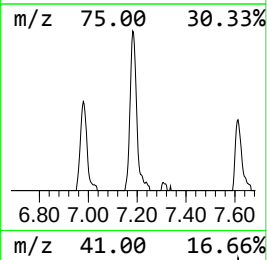
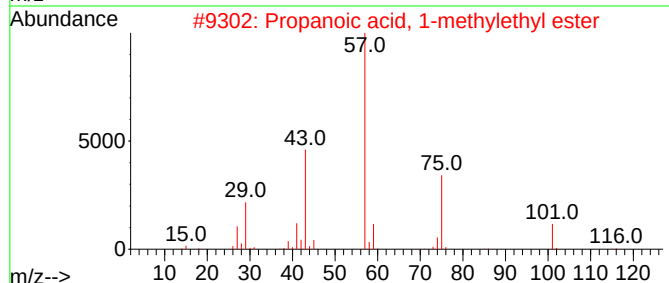
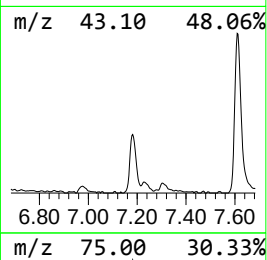
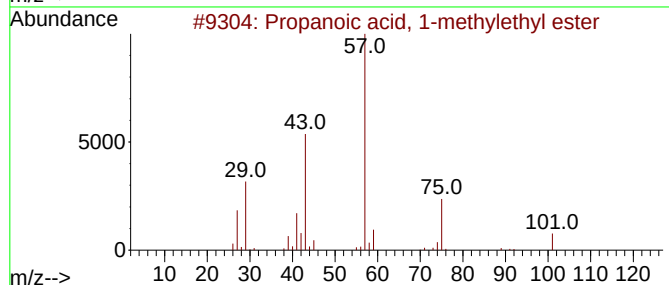
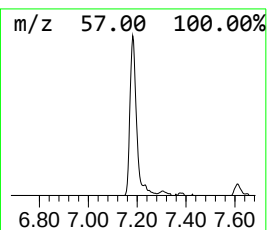
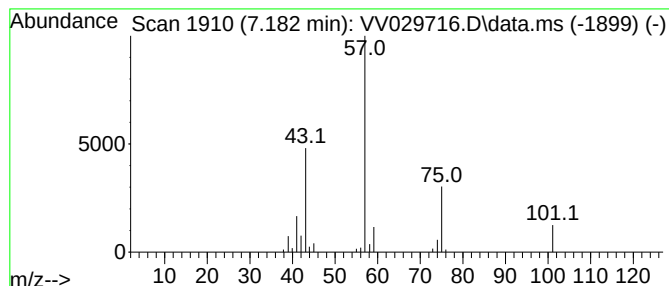
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.182	2.68 ug/L	55745	1,4-Difluorobenzene	5.609

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53



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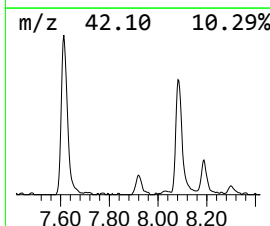
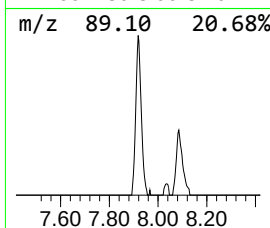
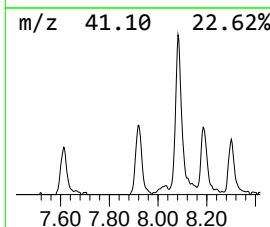
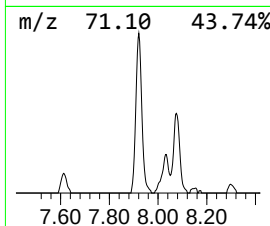
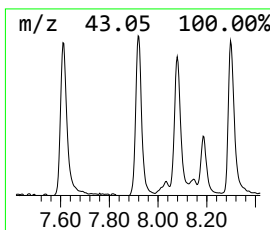
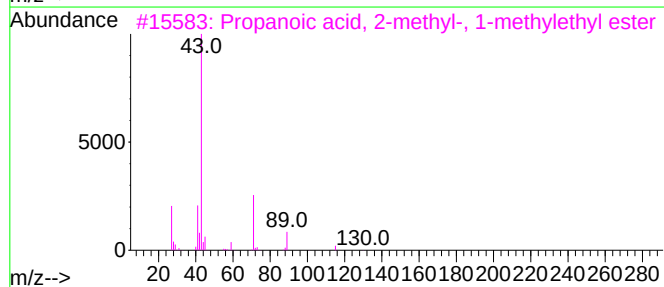
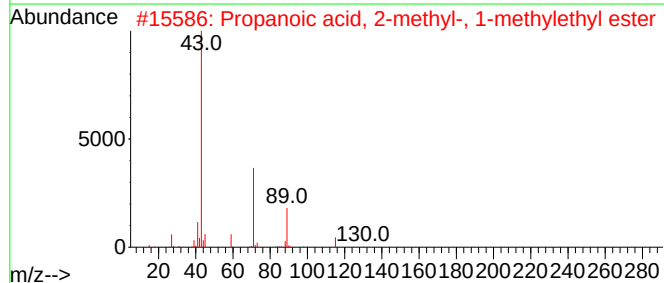
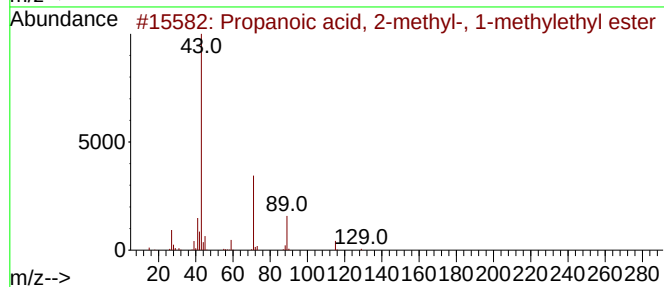
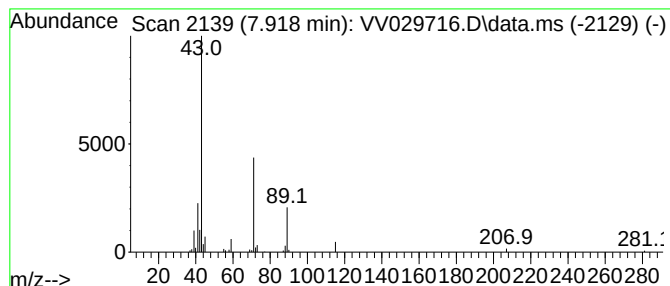
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Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.918	2.77 ug/L	69977	Chlorobenzene-d5	8.844

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029716.D
Acq On : 19 Dec 2022 13:05
Operator : SY/MD
Sample : N6075-06 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM0

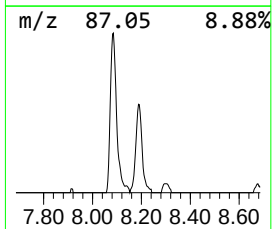
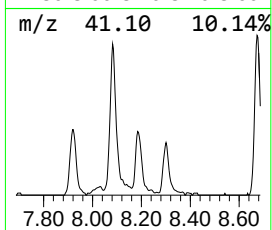
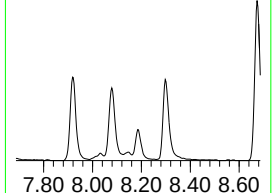
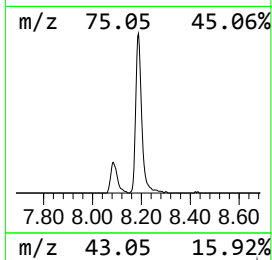
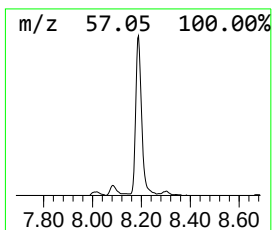
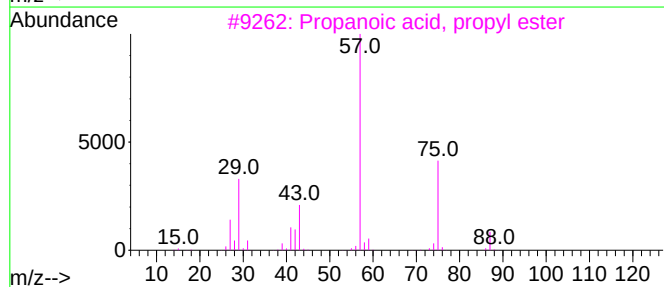
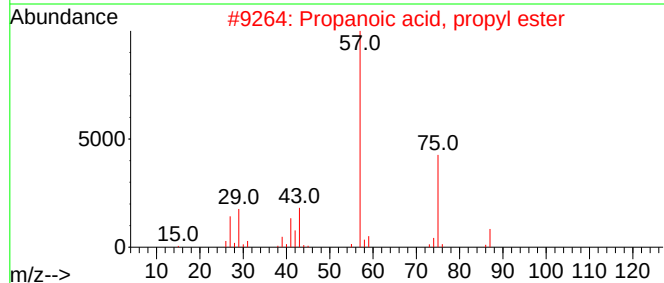
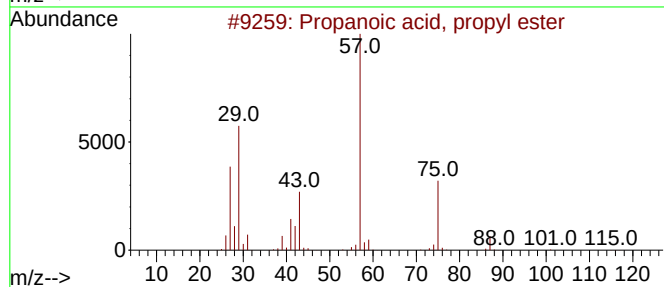
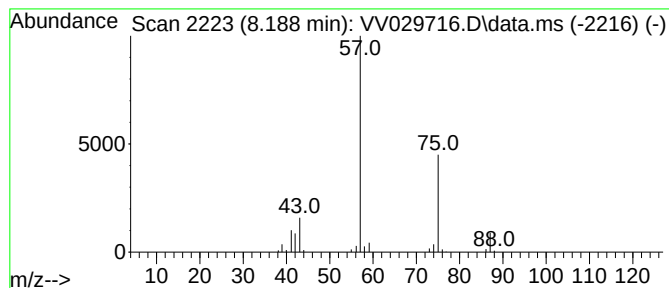
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.188	4.75 ug/L	119763	Chlorobenzene-d5	8.844

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029716.D
Acq On : 19 Dec 2022 13:05
Operator : SY/MD
Sample : N6075-06 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM0

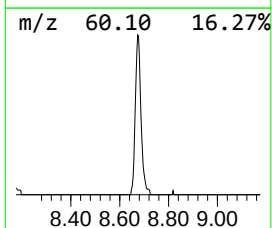
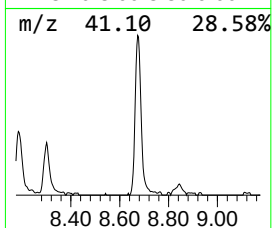
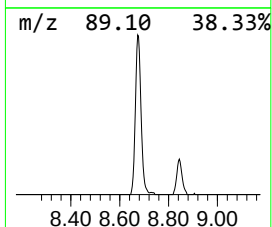
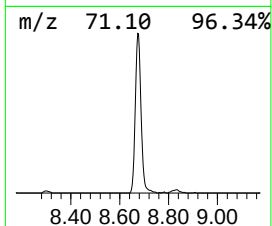
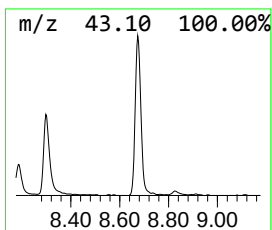
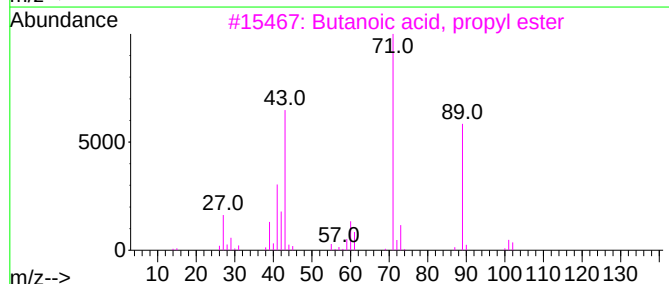
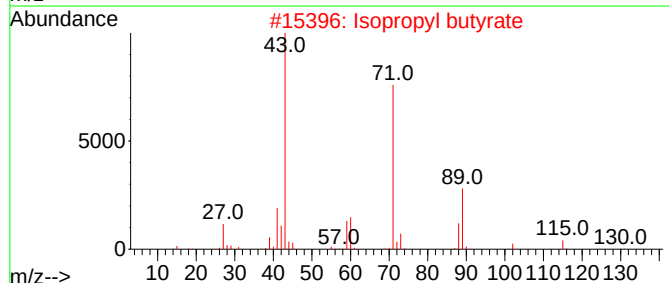
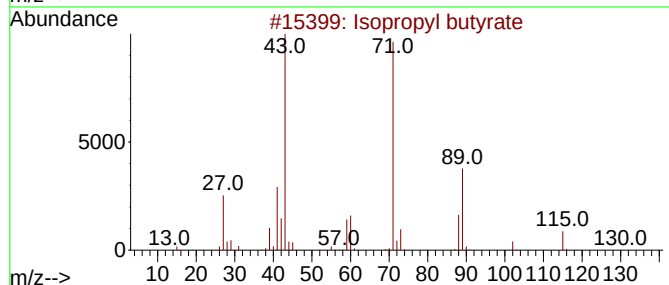
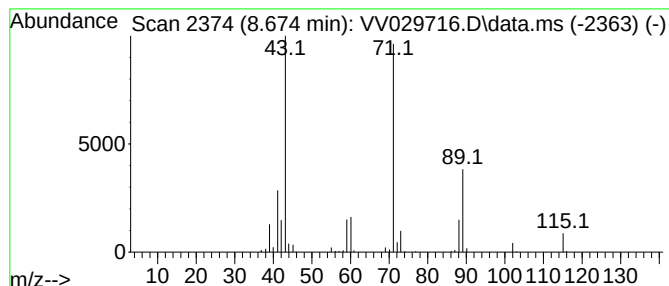
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.674	7.99 ug/L	201504	Chlorobenzene-d5	8.844

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029716.D
Acq On : 19 Dec 2022 13:05
Operator : SY/MD
Sample : N6075-06 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.461	12.6	ug/L	262666	1	5.609	1039720	50.0
Propanoic acid,...	7.182	2.7	ug/L	55745	1	5.609	1039720	50.0
Propanoic acid,...	7.918	2.8	ug/L	69977	2	8.844	1261580	50.0
Propanoic acid,...	8.188	4.8	ug/L	119763	2	8.844	1261580	50.0
Isopropyl butyrate	8.674	8.0	ug/L	201504	2	8.844	1261580	50.0