

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
 Data File : VV029720.D
 Acq On : 19 Dec 2022 14:39
 Operator : SY/MD
 Sample : N6075-10 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGSM6

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: VV029720.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	75	82	94	rVB	210977	205612	15.01%	1.703%
2	1.565	155	163	176	rVB	168774	188277	13.74%	1.559%
3	2.105	320	331	343	rBV	330972	471793	34.43%	3.907%
4	2.372	412	414	422	rVB2	299	261	0.02%	0.002%
5	2.503	445	455	468	rVB2	7832	12898	0.94%	0.107%
6	2.619	484	491	494	rBV2	477	740	0.05%	0.006%
7	2.693	509	514	519	rBV2	248	214	0.02%	0.002%
8	2.957	592	596	599	rBV2	158	174	0.01%	0.001%
9	3.182	659	666	669	rBV4	754	888	0.06%	0.007%
10	3.873	871	881	920	rBV2	90912	275173	20.08%	2.279%
11	4.249	991	998	1001	rBV4	289	364	0.03%	0.003%
12	4.269	1002	1004	1008	rVB3	485	312	0.02%	0.003%
13	4.339	1008	1026	1058	rBV	212385	532790	38.88%	4.412%
14	4.587	1099	1103	1106	rVB4	298	227	0.02%	0.002%
15	4.616	1110	1112	1115	rVB2	361	196	0.01%	0.002%
16	4.683	1130	1133	1138	rVB3	237	203	0.01%	0.002%
17	4.732	1140	1148	1150	rBV2	231	269	0.02%	0.002%
18	4.770	1155	1160	1164	rBV2	192	193	0.01%	0.002%
19	4.947	1207	1215	1216	rBV	266	227	0.02%	0.002%
20	5.040	1226	1244	1276	rBV2	519566	1370184	100.00%	11.346%
21	5.285	1308	1320	1343	rBV3	10454	26230	1.91%	0.217%
22	5.394	1352	1354	1359	rVB3	658	434	0.03%	0.004%
23	5.462	1372	1375	1378	rBV2	469	315	0.02%	0.003%
24	5.609	1408	1421	1458	rBV	494762	1015031	74.08%	8.405%
25	5.899	1502	1511	1525	rVB3	4630	9839	0.72%	0.081%
26	5.973	1531	1534	1539	rVB3	381	388	0.03%	0.003%
27	6.063	1547	1562	1599	rBV	296182	616632	45.00%	5.106%
28	6.262	1622	1624	1628	rVB3	616	400	0.03%	0.003%
29	6.288	1628	1632	1637	rBV3	282	273	0.02%	0.002%
30	6.352	1642	1652	1675	rBV2	4057	12578	0.92%	0.104%
31	6.461	1676	1686	1720	rBV	126329	249015	18.17%	2.062%
32	6.600	1727	1729	1731	rBV3	583	299	0.02%	0.002%
33	6.924	1823	1830	1833	rBV3	227	255	0.02%	0.002%
34	6.979	1833	1847	1874	rBV	150643	282896	20.65%	2.343%
35	7.114	1886	1889	1892	rVB3	366	236	0.02%	0.002%
36	7.182	1898	1910	1922	rBV	29451	53242	3.89%	0.441%

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Integrator: RTE

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

37	7.307	1936	1949	1982	rBV	641979	1143773	83.48%	9.471%
38	7.571	2028	2031	2033	rBV3	432	255	0.02%	0.002%
39	7.613	2033	2044	2066	rBV	141350	253578	18.51%	2.100%
40	7.773	2092	2094	2100	rVB3	424	344	0.03%	0.003%
41	7.921	2129	2140	2155	rVV	38775	66815	4.88%	0.553%
42	8.031	2162	2174	2180	rBV6	6791	12615	0.92%	0.104%
43	8.082	2180	2190	2213	rVV	326594	597852	43.63%	4.951%
44	8.185	2215	2222	2240	rVB	66127	111644	8.15%	0.924%
45	8.297	2249	2257	2278	rVB	39796	66213	4.83%	0.548%
46	8.471	2308	2311	2314	rBV2	389	382	0.03%	0.003%
47	8.497	2318	2319	2323	rVB3	399	210	0.02%	0.002%
48	8.519	2323	2326	2329	rVB	283	185	0.01%	0.002%
49	8.551	2333	2336	2341	rVB2	523	348	0.03%	0.003%
50	8.574	2341	2343	2348	rVB3	296	178	0.01%	0.001%
51	8.616	2348	2356	2357	rBV3	256	281	0.02%	0.002%
52	8.674	2361	2374	2398	rBV	118961	189841	13.86%	1.572%
53	8.844	2414	2427	2457	rBV	737701	1224561	89.37%	10.140%
54	8.995	2472	2474	2476	rBV2	367	179	0.01%	0.001%
55	9.108	2499	2509	2511	rBV7	1321	1697	0.12%	0.014%
56	9.211	2538	2541	2545	rVB2	410	252	0.02%	0.002%
57	9.252	2552	2554	2559	rVB2	239	196	0.01%	0.002%
58	9.387	2588	2596	2600	rBV3	1177	1809	0.13%	0.015%
59	9.423	2605	2607	2613	rVB2	327	259	0.02%	0.002%
60	9.542	2635	2644	2656	rBV3	9824	15470	1.13%	0.128%
61	9.751	2708	2709	2714	rVB2	351	222	0.02%	0.002%
62	9.818	2727	2730	2736	rBV3	271	265	0.02%	0.002%
63	9.921	2757	2762	2763	rBV	389	313	0.02%	0.003%
64	9.957	2770	2773	2776	rVB2	251	175	0.01%	0.001%
65	10.162	2828	2837	2840	rVV	15740	20780	1.52%	0.172%
66	10.204	2841	2850	2878	rVV	427974	674469	49.22%	5.585%
67	10.310	2881	2883	2888	rVV3	469	322	0.02%	0.003%
68	10.371	2895	2902	2910	rBV4	1731	2221	0.16%	0.018%
69	10.526	2946	2950	2954	rVV3	329	397	0.03%	0.003%
70	10.567	2954	2963	2976	rVB3	7607	12200	0.89%	0.101%
71	10.619	2976	2979	2984	rBV3	265	193	0.01%	0.002%
72	10.654	2984	2990	2994	rVB2	270	291	0.02%	0.002%
73	10.686	2995	3000	3004	rBV2	218	265	0.02%	0.002%
74	10.863	3053	3055	3063	rVB2	202	225	0.02%	0.002%
75	10.918	3070	3072	3074	rVB	465	187	0.01%	0.002%
76	10.937	3074	3078	3085	rBV2	376	281	0.02%	0.002%

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 Title : VOC Analysis

77	11.037	3105	3109	3114	rBV3	340	387	0.03%	0.003%
78	11.172	3147	3151	3152	rBV2	320	222	0.02%	0.002%
79	11.236	3159	3171	3199	rBV	817988	1256610	91.71%	10.406%
80	11.384	3215	3217	3224	rVB2	607	529	0.04%	0.004%
81	11.416	3224	3227	3232	rVB2	537	437	0.03%	0.004%
82	11.455	3234	3239	3242	rVB2	311	245	0.02%	0.002%
83	11.558	3267	3271	3275	rBV2	367	317	0.02%	0.003%
84	11.612	3275	3288	3313	rBV	685394	1080813	78.88%	8.950%
85	11.908	3378	3380	3383	rVV2	329	209	0.02%	0.002%
86	11.934	3385	3388	3392	rVB3	285	204	0.01%	0.002%
87	12.236	3478	3482	3484	rBV2	1227	898	0.07%	0.007%
88	12.413	3535	3537	3540	rVB2	316	178	0.01%	0.001%
89	12.429	3540	3542	3547	rBV2	427	267	0.02%	0.002%
90	12.706	3625	3628	3635	rBV2	437	506	0.04%	0.004%
91	12.805	3656	3659	3663	rBV3	320	255	0.02%	0.002%
92	12.895	3684	3687	3692	rBV4	374	392	0.03%	0.003%
93	12.953	3702	3705	3709	rVB2	422	333	0.02%	0.003%
94	13.024	3724	3727	3731	rVB3	416	314	0.02%	0.003%
95	13.085	3744	3746	3748	rBV	378	223	0.02%	0.002%
96	13.249	3793	3797	3802	rBV4	639	605	0.04%	0.005%
97	13.349	3826	3828	3831	rBV3	493	434	0.03%	0.004%
98	13.390	3836	3841	3843	rBV2	471	377	0.03%	0.003%
99	13.734	3945	3948	3950	rBV3	534	345	0.03%	0.003%
100	13.876	3990	3992	3997	rVB3	652	409	0.03%	0.003%

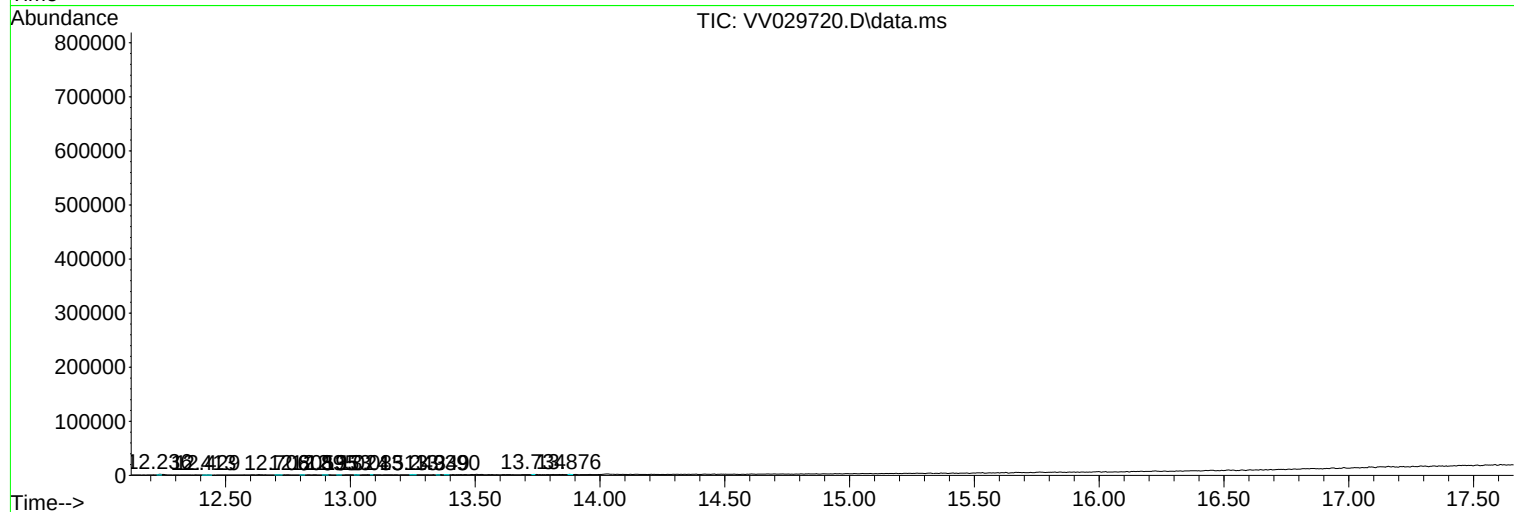
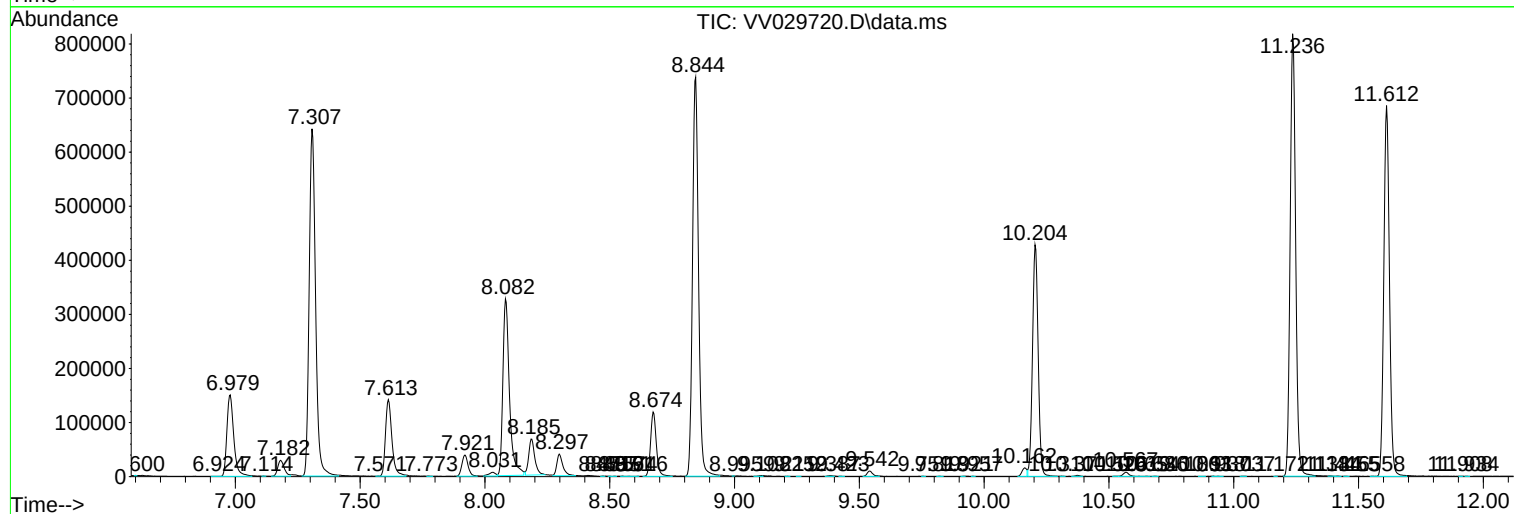
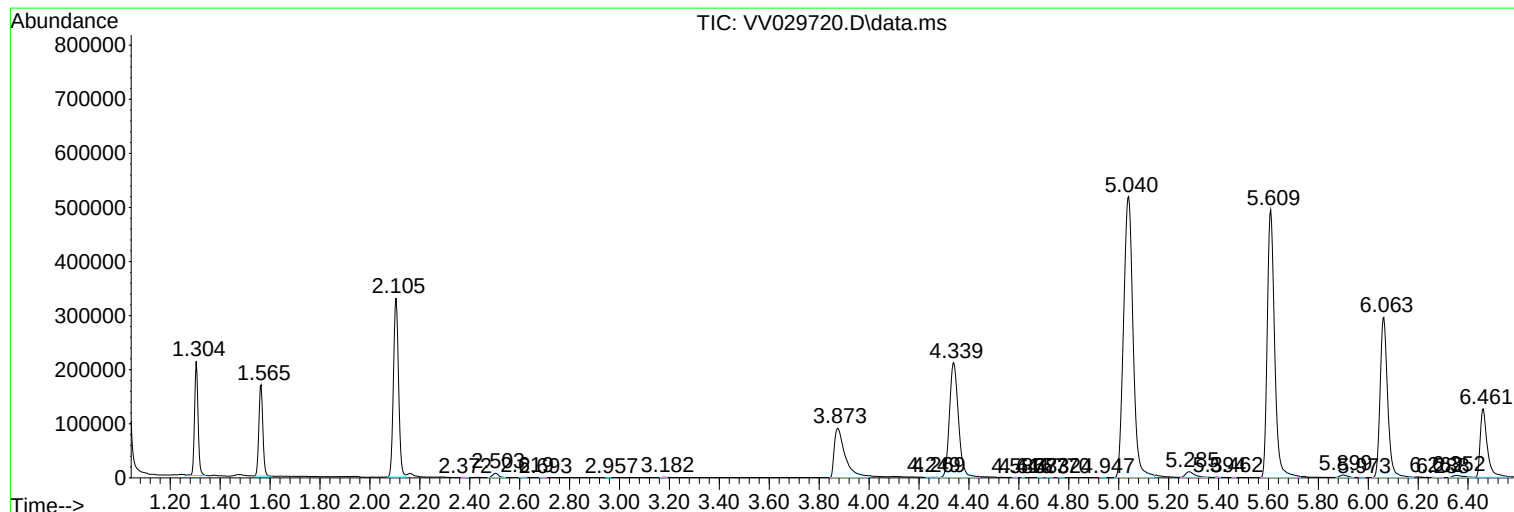
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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



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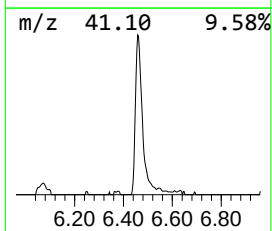
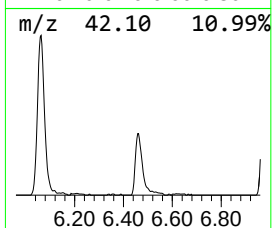
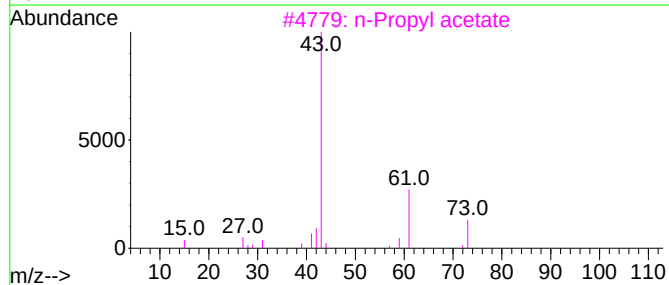
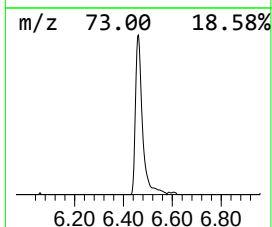
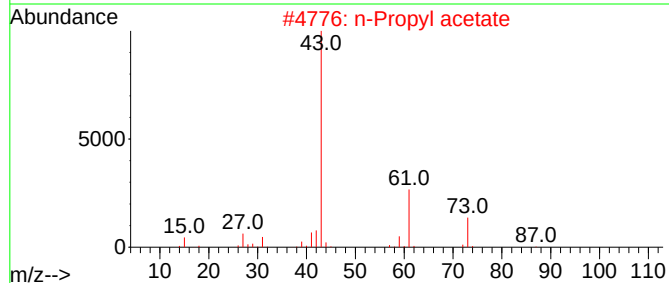
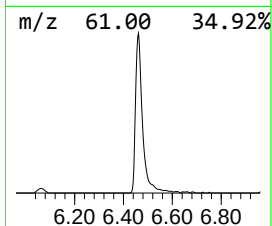
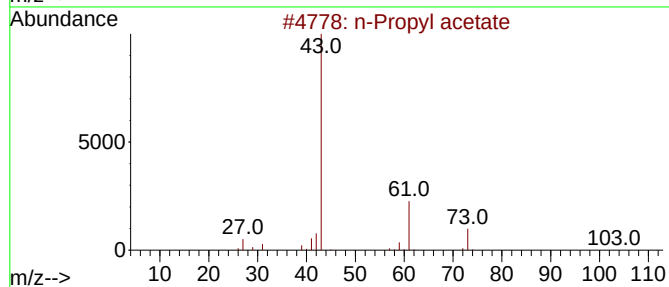
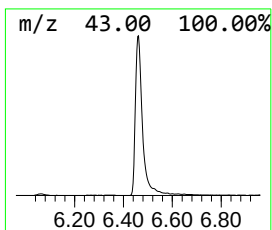
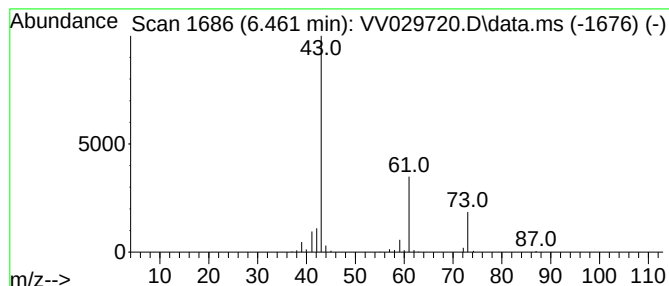
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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	12.27 ug/L	249015	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	83	
3	n-Propyl acetate	102	C5H10O2	000109-60-4	78	
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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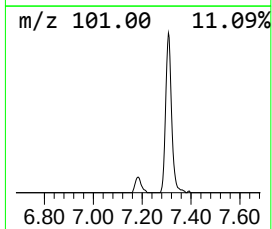
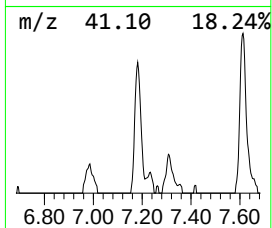
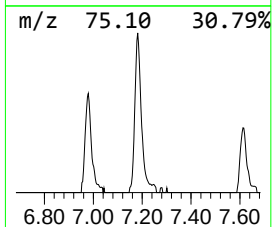
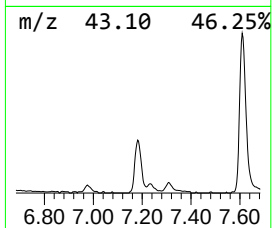
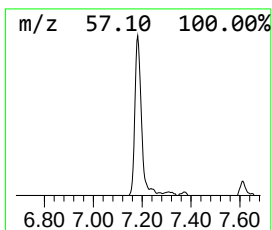
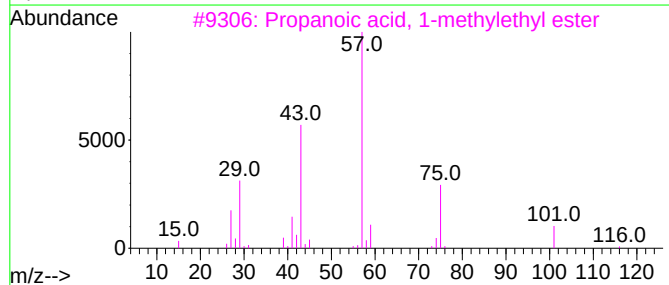
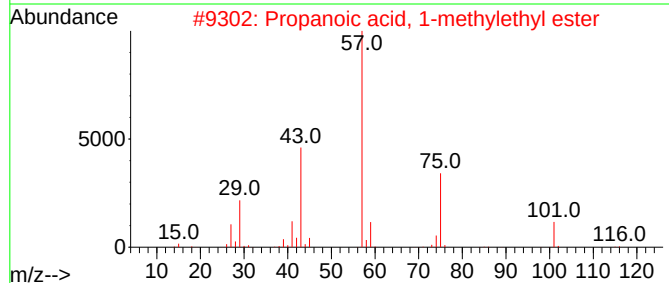
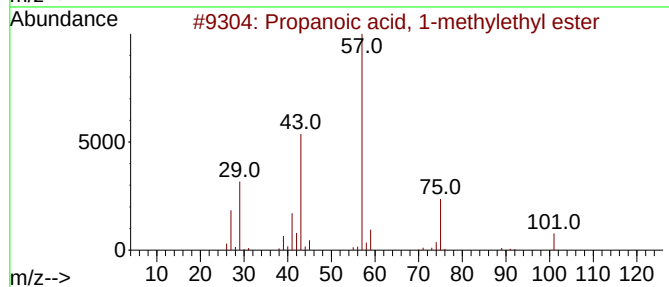
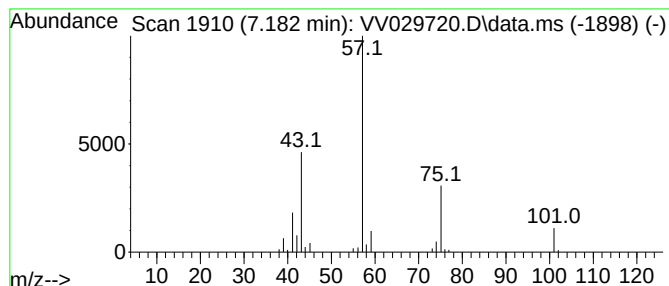
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.182	2.62 ug/L	53242	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	83
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53



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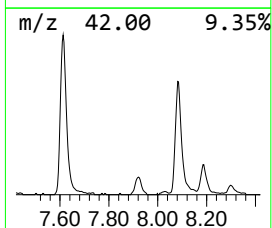
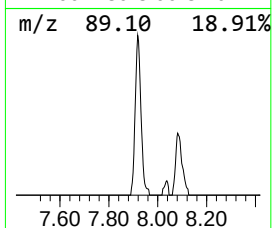
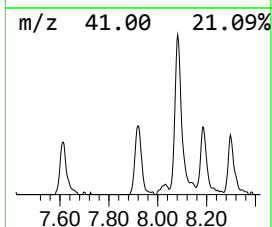
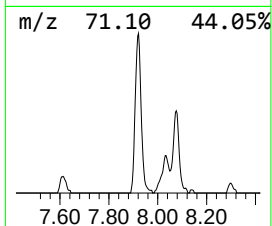
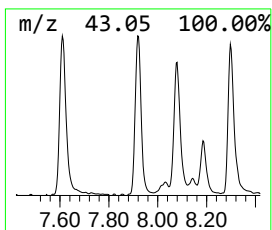
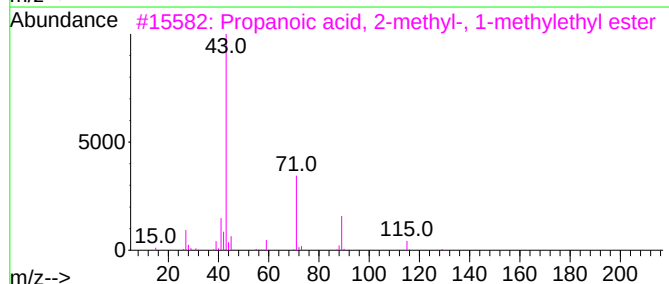
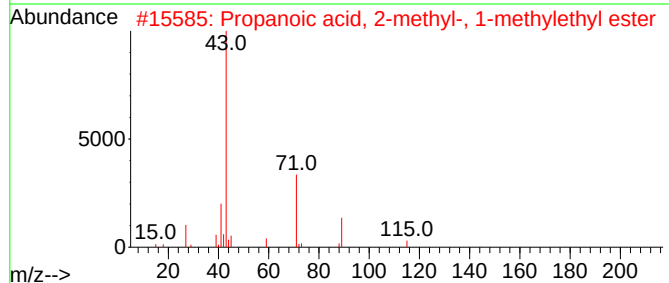
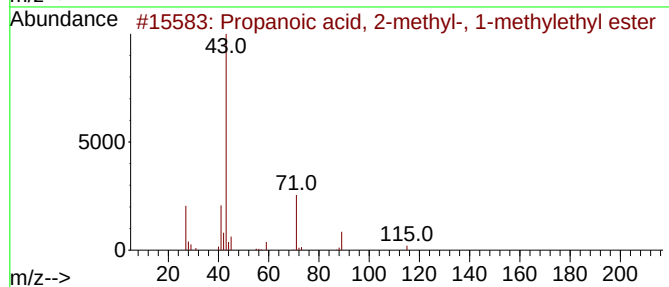
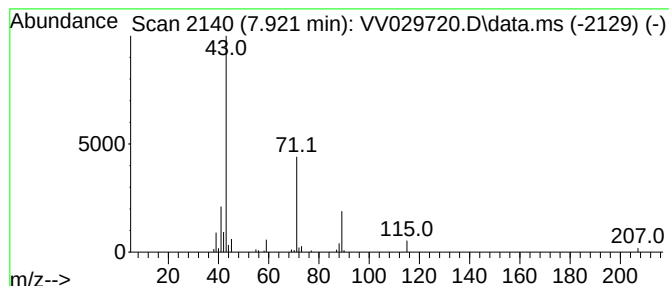
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.921	2.73 ug/L	66815	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	83
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
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	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029720.D
Acq On : 19 Dec 2022 14:39
Operator : SY/MD
Sample : N6075-10 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM6

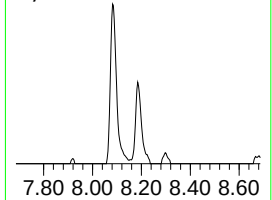
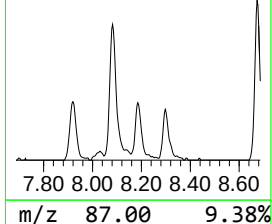
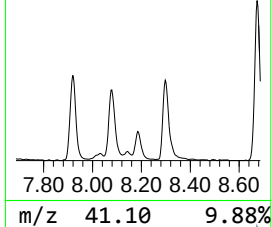
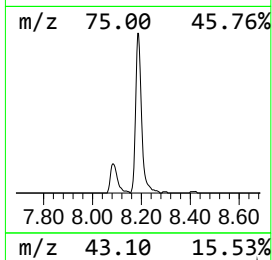
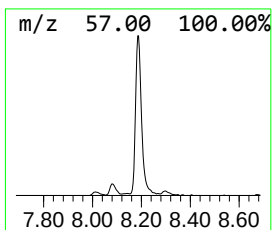
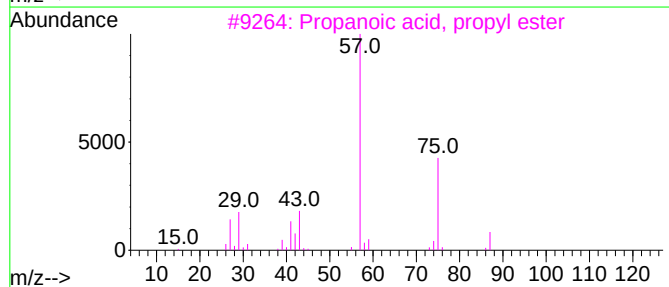
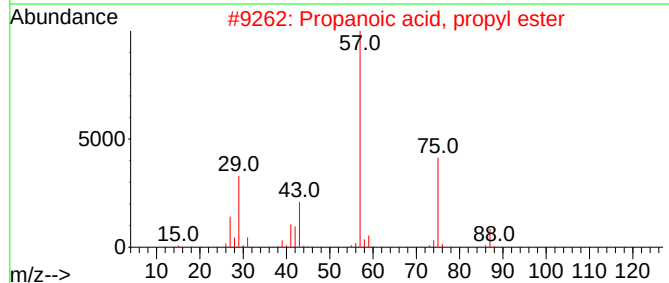
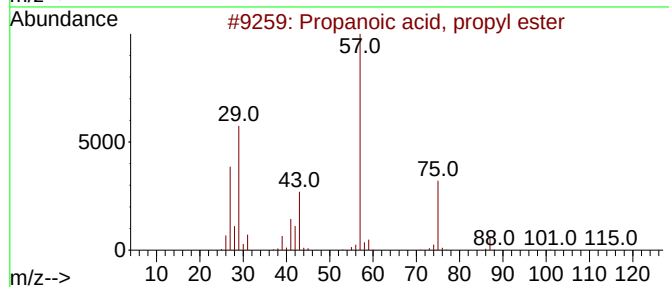
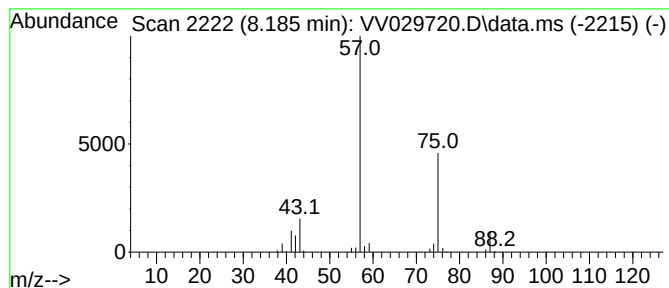
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Quant Title : VOC Analysis

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.
8.185	4.56 ug/L	111644	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	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029720.D
Acq On : 19 Dec 2022 14:39
Operator : SY/MD
Sample : N6075-10 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM6

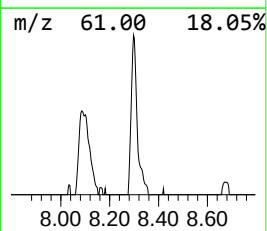
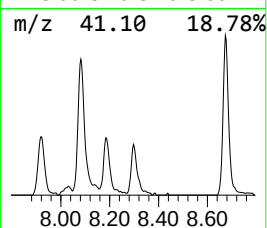
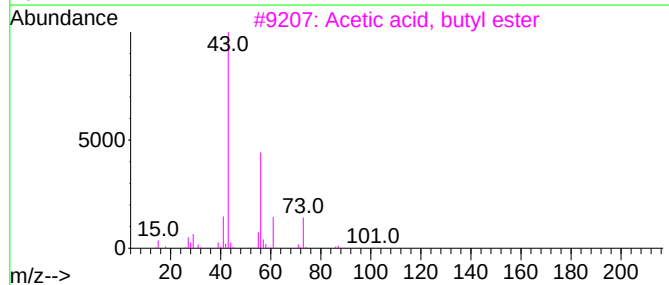
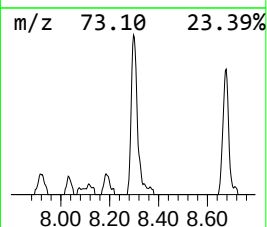
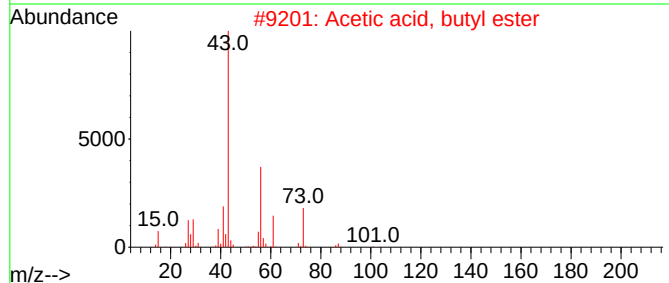
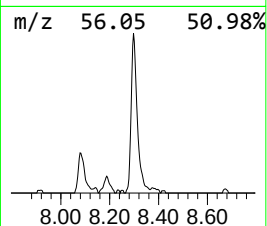
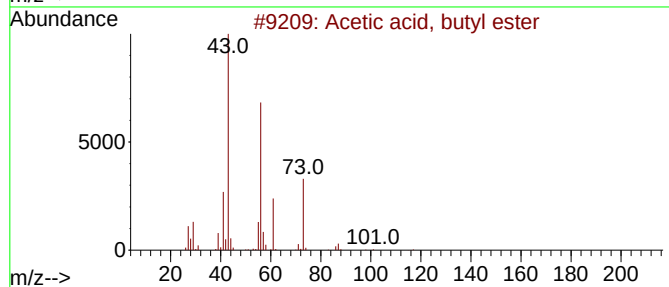
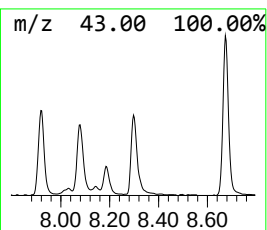
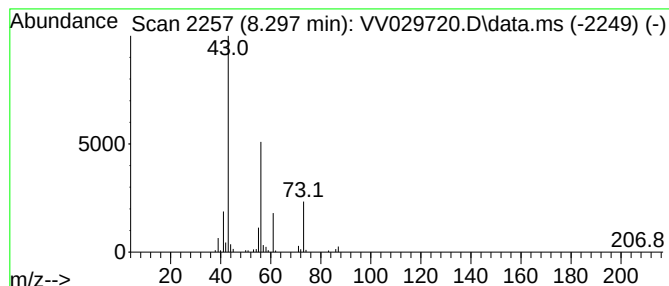
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.297	2.70 ug/L	66213	Chlorobenzene-d5	8.844

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78		
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78		
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72		
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64		
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	40		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029720.D
Acq On : 19 Dec 2022 14:39
Operator : SY/MD
Sample : N6075-10 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM6

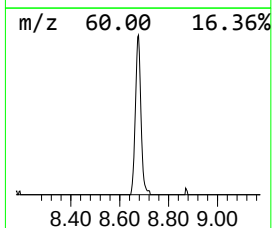
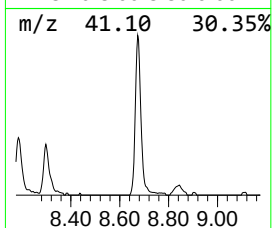
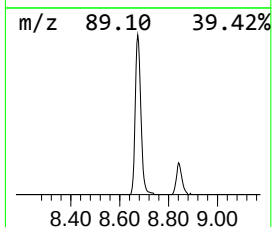
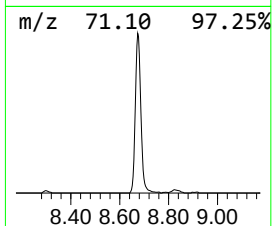
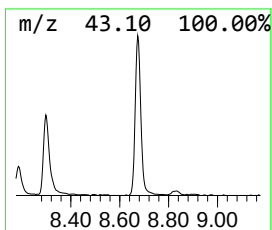
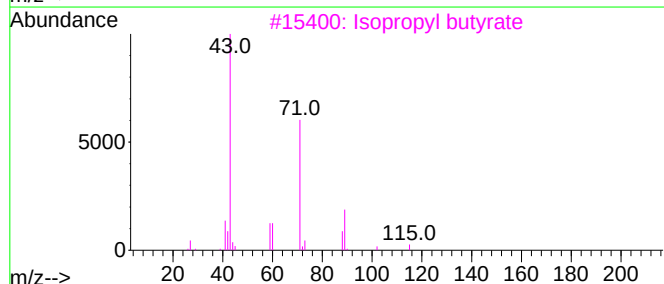
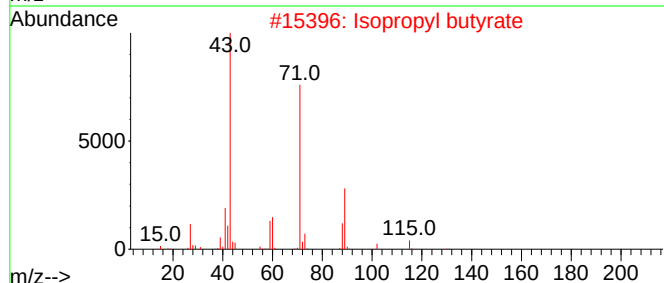
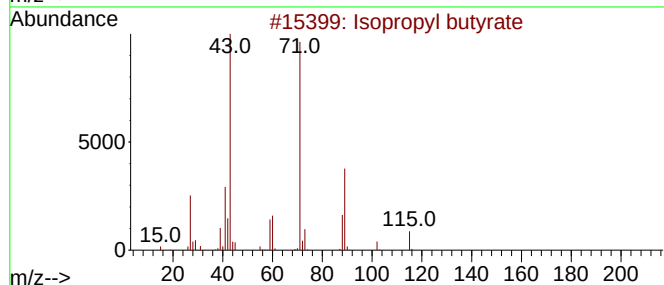
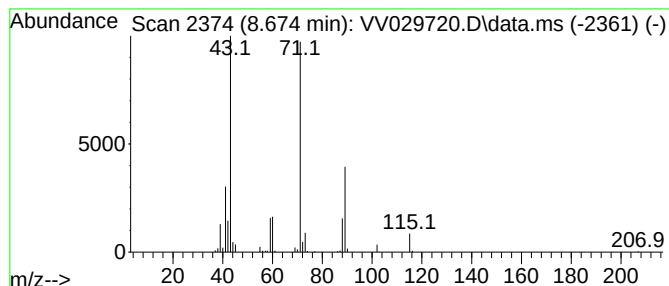
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.674	7.75 ug/L	189841	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			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029720.D
Acq On : 19 Dec 2022 14:39
Operator : SY/MD
Sample : N6075-10 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM6

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	12.3	ug/L	249015	1	5.609	1015030	50.0
Propanoic acid,...	7.182	2.6	ug/L	53242	1	5.609	1015030	50.0
Propanoic acid,...	7.921	2.7	ug/L	66815	2	8.844	1224560	50.0
Propanoic acid,...	8.185	4.6	ug/L	111644	2	8.844	1224560	50.0
Acetic acid, bu...	8.297	2.7	ug/L	66213	2	8.844	1224560	50.0
Isopropyl butyrate	8.674	7.8	ug/L	189841	2	8.844	1224560	50.0