

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
 Data File : VV029713.D
 Acq On : 19 Dec 2022 11:55
 Operator : SY/MD
 Sample : N6075-02 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGSM1

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: VV029713.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	99	rVB	221281	221179	15.50%	1.741%
2	1.564	155	163	175	rVB	169862	194557	13.64%	1.532%
3	1.947	280	282	288	rVB3	675	546	0.04%	0.004%
4	1.976	288	291	292	rBV	471	240	0.02%	0.002%
5	2.105	320	331	343	rBV	348068	498595	34.95%	3.926%
6	2.288	382	388	389	rBV4	607	527	0.04%	0.004%
7	2.433	428	433	442	rBV3	337	613	0.04%	0.005%
8	2.503	446	455	467	rVB2	9375	15559	1.09%	0.123%
9	2.622	490	492	496	rVB3	293	185	0.01%	0.001%
10	2.799	544	547	554	rBV2	383	312	0.02%	0.002%
11	2.953	592	595	600	rBV2	274	216	0.02%	0.002%
12	3.008	607	612	616	rVB2	193	192	0.01%	0.002%
13	3.060	623	628	630	rBV2	278	179	0.01%	0.001%
14	3.179	658	665	682	rVV5	1200	2864	0.20%	0.023%
15	3.429	739	743	748	rVV2	172	186	0.01%	0.001%
16	3.873	870	881	922	rBV2	95934	296285	20.77%	2.333%
17	4.275	1000	1006	1009	rBV3	326	324	0.02%	0.003%
18	4.339	1009	1026	1065	rBV	221523	551392	38.65%	4.341%
19	4.526	1082	1084	1088	rVB4	387	264	0.02%	0.002%
20	4.641	1116	1120	1123	rVB3	409	346	0.02%	0.003%
21	4.667	1124	1128	1131	rBV2	394	322	0.02%	0.003%
22	4.693	1131	1136	1140	rVB4	360	327	0.02%	0.003%
23	5.040	1225	1244	1290	rBV2	538964	1426784	100.00%	11.234%
24	5.281	1309	1319	1335	rBV3	11377	26407	1.85%	0.208%
25	5.394	1352	1354	1361	rVB2	470	443	0.03%	0.003%
26	5.461	1372	1375	1377	rBV2	226	173	0.01%	0.001%
27	5.558	1401	1405	1408	rBV3	225	211	0.01%	0.002%
28	5.609	1408	1421	1465	rBV	518030	1060856	74.35%	8.353%
29	5.902	1501	1512	1526	rBV6	5090	10871	0.76%	0.086%
30	6.063	1548	1562	1595	rBV	302644	633855	44.43%	4.991%
31	6.236	1614	1616	1620	rVB2	433	253	0.02%	0.002%
32	6.294	1629	1634	1636	rBV2	338	342	0.02%	0.003%
33	6.346	1641	1650	1652	rBV	4876	5344	0.37%	0.042%
34	6.458	1676	1685	1718	rBV	147874	289519	20.29%	2.280%
35	6.731	1769	1770	1778	rVB2	359	284	0.02%	0.002%
36	6.979	1833	1847	1878	rBV	156240	292098	20.47%	2.300%

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Integrator: RTE

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

37	7.182	1899	1910	1922	rBV	34710	60005	4.21%	0.472%
38	7.307	1937	1949	1986	rBV	668240	1193946	83.68%	9.401%
39	7.522	2014	2016	2021	rVB2	500	341	0.02%	0.003%
40	7.612	2033	2044	2073	rBV2	149501	268168	18.80%	2.111%
41	7.796	2099	2101	2105	rVB3	715	477	0.03%	0.004%
42	7.863	2118	2122	2125	rVB3	438	337	0.02%	0.003%
43	7.921	2129	2140	2160	rBV2	42126	73839	5.18%	0.581%
44	8.030	2160	2174	2180	rBV5	8368	16284	1.14%	0.128%
45	8.082	2180	2190	2214	rVV	351143	649355	45.51%	5.113%
46	8.188	2215	2223	2241	rVB	74813	123992	8.69%	0.976%
47	8.297	2248	2257	2278	rVB	44289	77069	5.40%	0.607%
48	8.455	2304	2306	2311	rVB2	357	197	0.01%	0.002%
49	8.503	2318	2321	2324	rBV4	687	464	0.03%	0.004%
50	8.593	2347	2349	2352	rVB2	570	277	0.02%	0.002%
51	8.673	2363	2374	2401	rBV	131101	212443	14.89%	1.673%
52	8.783	2405	2408	2411	rVB2	449	214	0.01%	0.002%
53	8.844	2413	2427	2461	rBV	769590	1278986	89.64%	10.070%
54	9.011	2475	2479	2480	rBV3	407	341	0.02%	0.003%
55	9.053	2489	2492	2496	rBV4	632	443	0.03%	0.003%
56	9.111	2502	2510	2526	rVB6	2001	3941	0.28%	0.031%
57	9.387	2588	2596	2606	rVB3	1540	2630	0.18%	0.021%
58	9.448	2612	2615	2618	rBV2	215	187	0.01%	0.001%
59	9.542	2636	2644	2659	rVV2	10512	16420	1.15%	0.129%
60	9.638	2668	2674	2677	rBV2	198	192	0.01%	0.002%
61	9.767	2711	2714	2717	rBV3	193	172	0.01%	0.001%
62	9.850	2733	2740	2744	rVB2	200	236	0.02%	0.002%
63	9.889	2744	2752	2757	rBV3	249	410	0.03%	0.003%
64	9.918	2757	2761	2766	rVV2	394	503	0.04%	0.004%
65	10.162	2828	2837	2840	rBV2	16495	22096	1.55%	0.174%
66	10.207	2841	2851	2868	rVB	439543	690558	48.40%	5.437%
67	10.368	2895	2901	2903	rBV3	1370	1278	0.09%	0.010%
68	10.448	2921	2926	2929	rBV2	332	302	0.02%	0.002%
69	10.519	2942	2948	2949	rBV	360	268	0.02%	0.002%
70	10.567	2955	2963	2975	rVB2	7393	12248	0.86%	0.096%
71	10.905	3062	3068	3071	rBV3	385	381	0.03%	0.003%
72	11.085	3122	3124	3129	rBV2	250	228	0.02%	0.002%
73	11.146	3140	3143	3145	rBV	361	278	0.02%	0.002%
74	11.175	3148	3152	3157	rVB3	778	885	0.06%	0.007%
75	11.236	3157	3171	3195	rBV	849019	1326327	92.96%	10.443%
76	11.471	3243	3244	3249	rVB3	319	180	0.01%	0.001%

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77	11.535	3261	3264	3269	rVB	319	284	0.02%	0.002%
78	11.612	3275	3288	3316	rBV	714053	1117376	78.31%	8.798%
79	11.715	3316	3320	3323	rVB3	888	776	0.05%	0.006%
80	11.824	3352	3354	3358	rBV	314	317	0.02%	0.002%
81	11.866	3363	3367	3368	rBV	324	199	0.01%	0.002%
82	11.943	3387	3391	3394	rBV2	339	232	0.02%	0.002%
83	11.969	3395	3399	3401	rVV2	424	317	0.02%	0.002%
84	11.998	3405	3408	3411	rBV	324	219	0.02%	0.002%
85	12.146	3451	3454	3456	rVB2	389	234	0.02%	0.002%
86	12.239	3475	3483	3493	rBV3	1410	2489	0.17%	0.020%
87	12.294	3497	3500	3501	rBV	432	190	0.01%	0.001%
88	12.342	3513	3515	3517	rBV	445	225	0.02%	0.002%
89	12.632	3602	3605	3611	rVB4	626	656	0.05%	0.005%
90	12.722	3631	3633	3640	rVB2	629	576	0.04%	0.005%
91	12.754	3640	3643	3644	rBV3	318	175	0.01%	0.001%
92	13.091	3745	3748	3750	rBV2	275	201	0.01%	0.002%
93	13.255	3790	3799	3806	rBV6	984	1774	0.12%	0.014%
94	13.310	3814	3816	3821	rVB2	482	320	0.02%	0.003%
95	13.342	3821	3826	3829	rBV2	705	641	0.04%	0.005%
96	13.422	3848	3851	3854	rBV3	334	212	0.01%	0.002%
97	13.500	3868	3875	3882	rBV5	2057	2675	0.19%	0.021%
98	14.297	4121	4123	4126	rVB2	452	192	0.01%	0.002%
99	14.316	4126	4129	4130	rBV2	617	409	0.03%	0.003%
100	14.487	4180	4182	4183	rBV	561	265	0.02%	0.002%

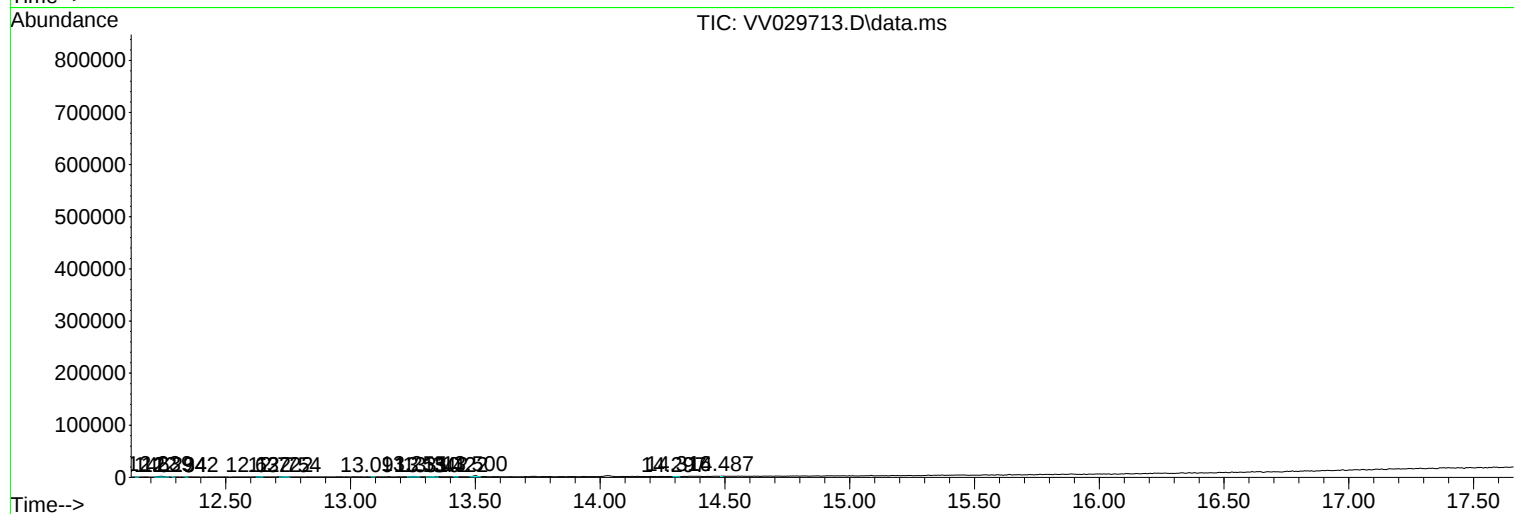
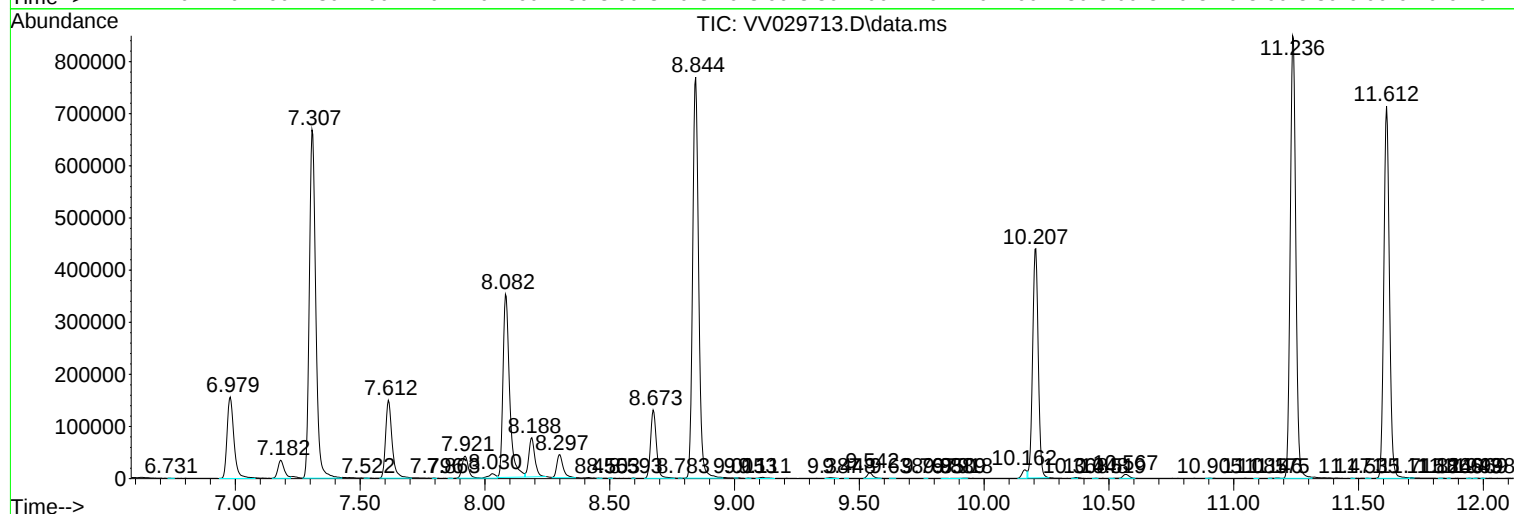
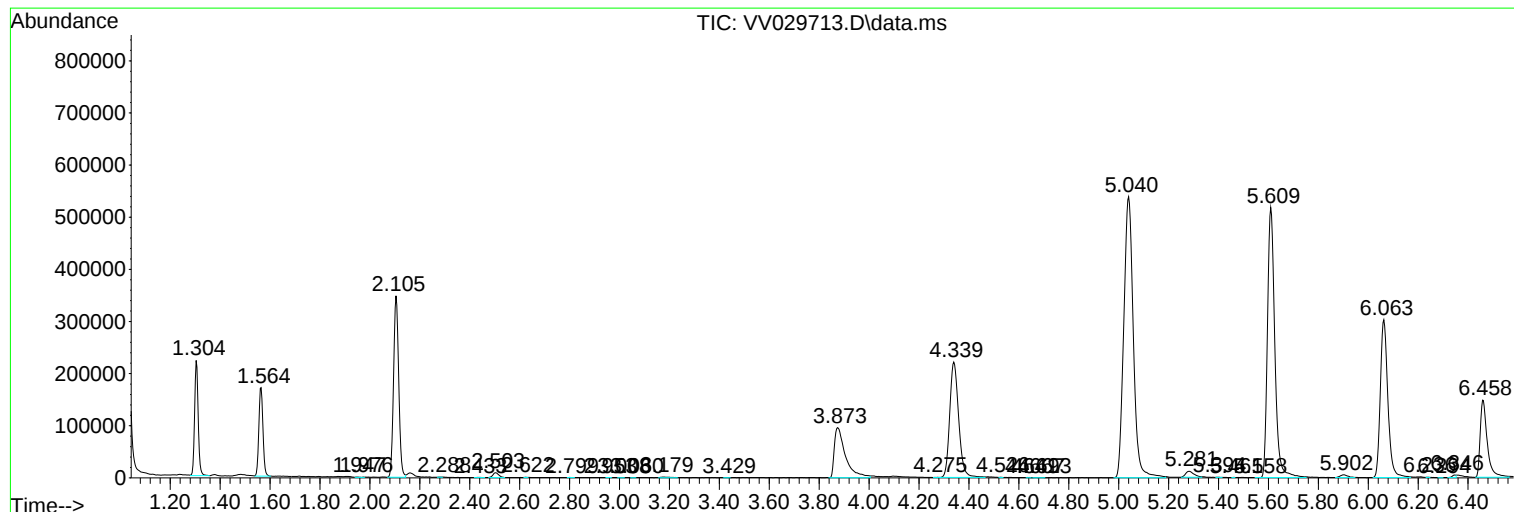
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Instrument :
MSVOA_V
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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



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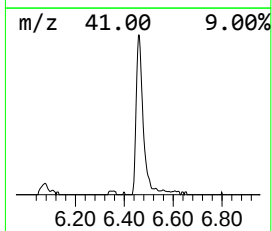
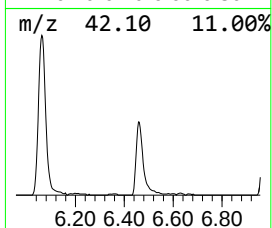
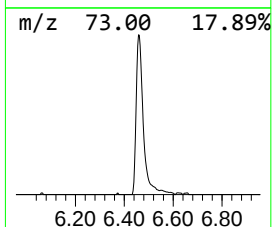
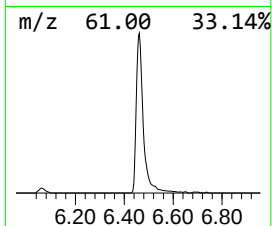
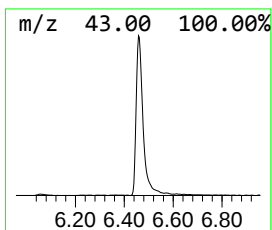
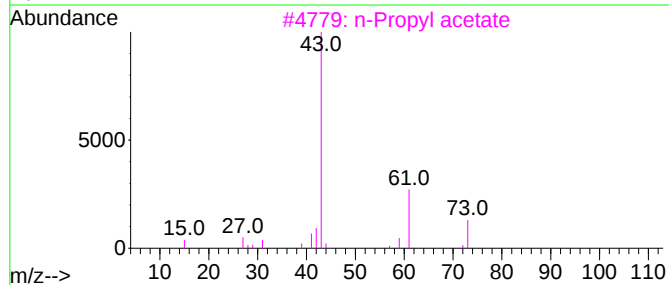
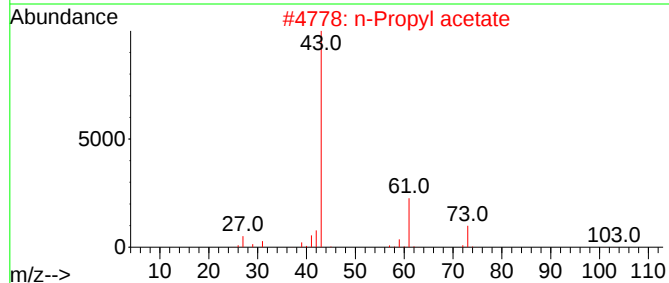
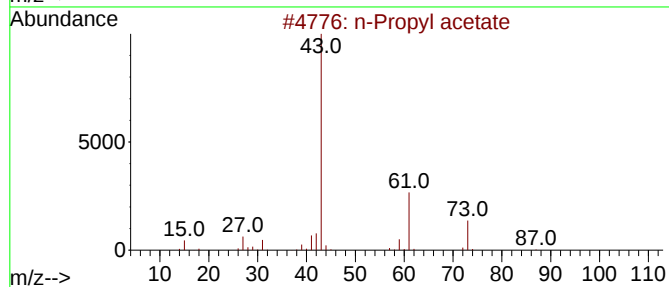
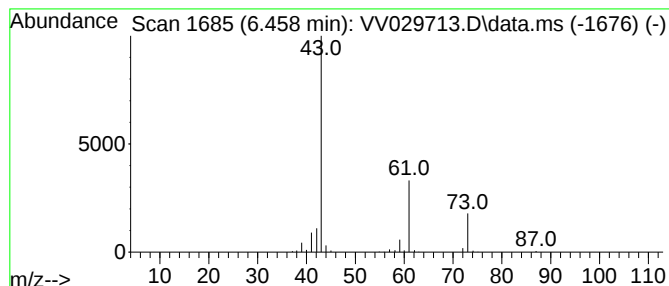
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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.
6.458	13.65 ug/L	289519	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	Isopropyl acetate			102	C5H10O2	000108-21-4	36



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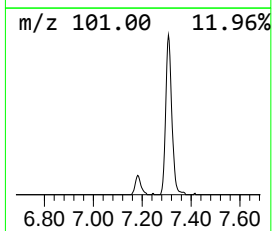
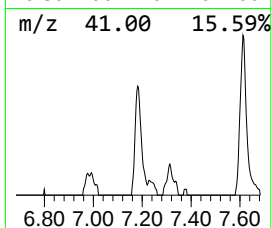
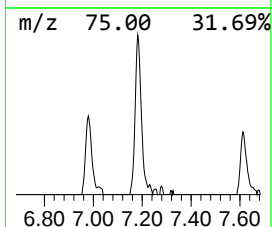
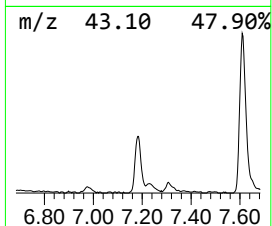
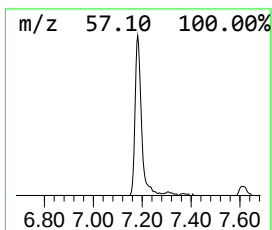
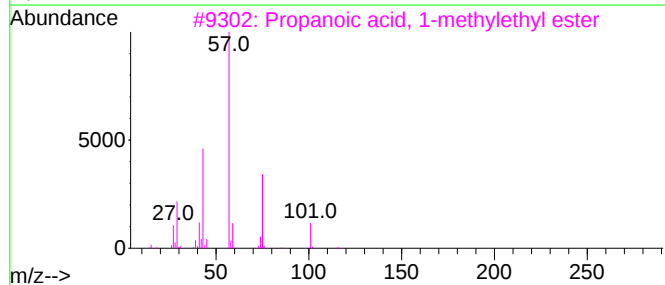
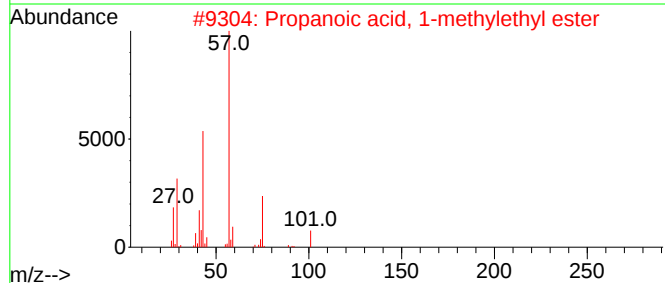
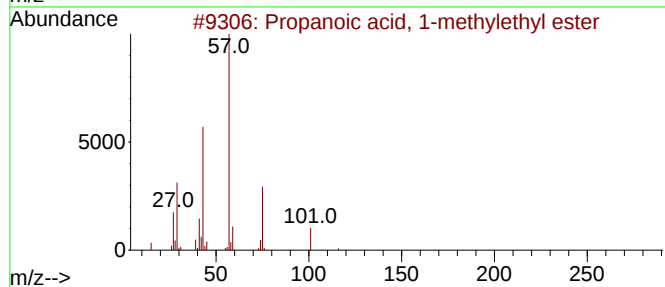
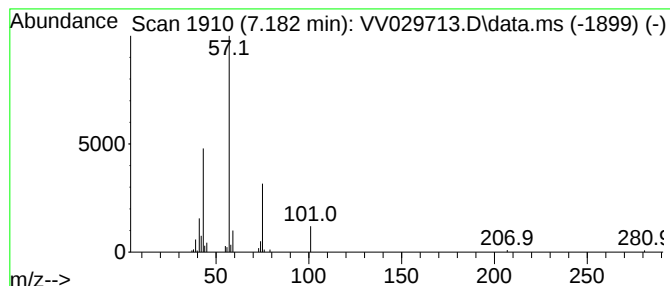
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.182	2.83 ug/L	60005	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	78
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53



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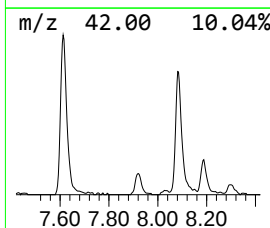
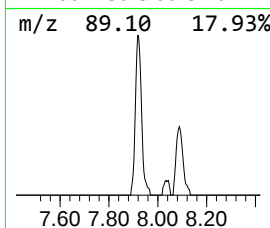
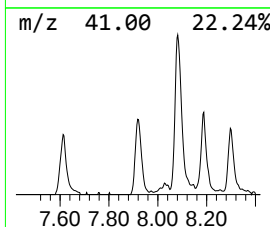
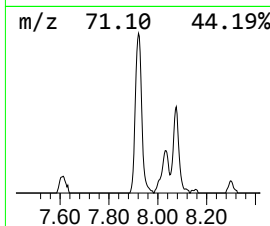
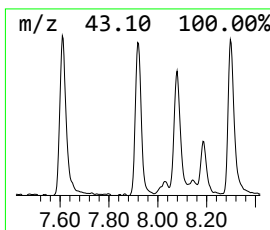
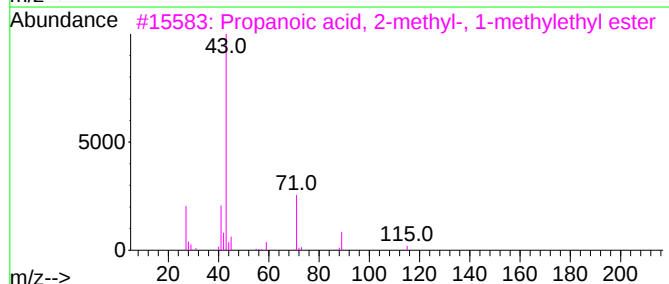
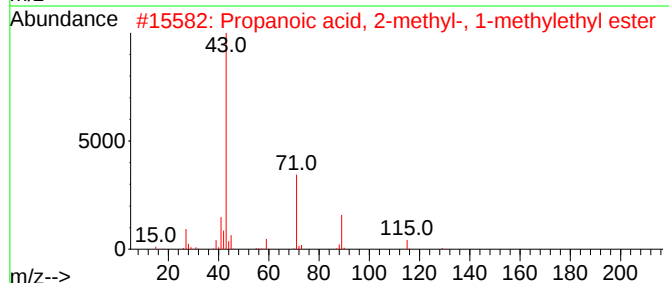
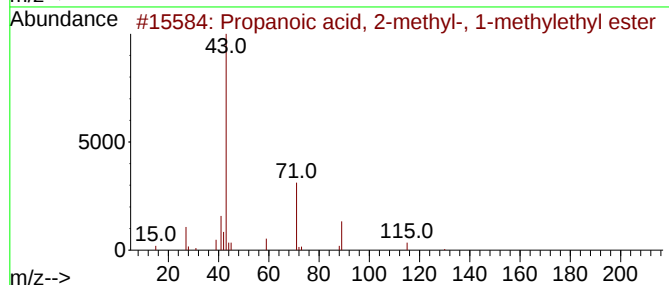
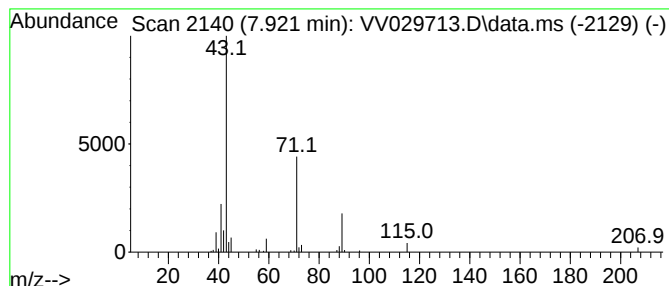
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.921	2.89 ug/L	73839	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	83
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029713.D
Acq On : 19 Dec 2022 11:55
Operator : SY/MD
Sample : N6075-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM1

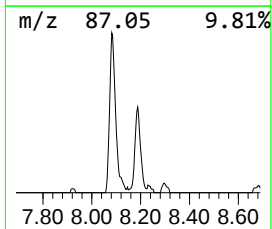
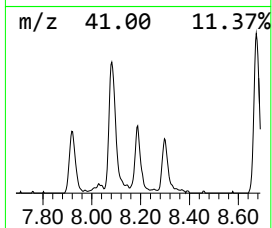
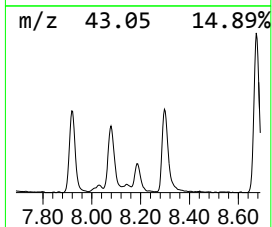
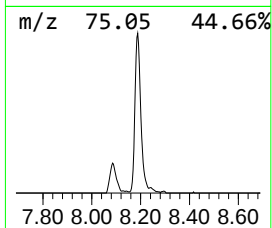
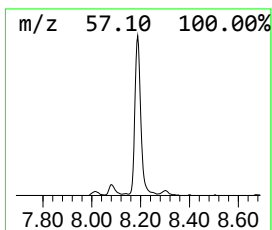
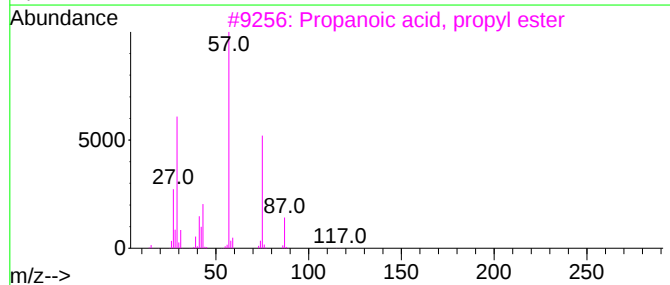
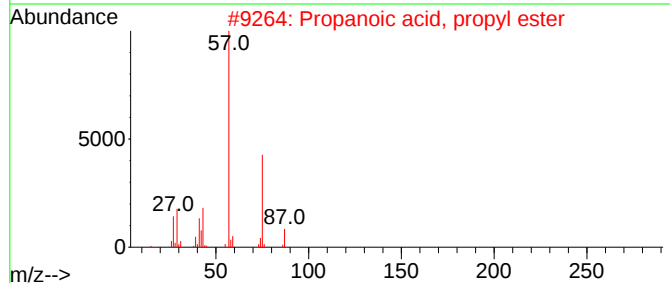
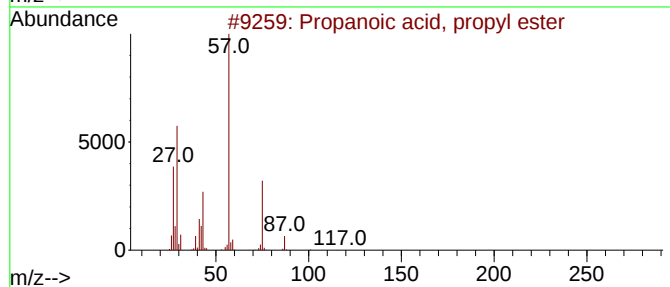
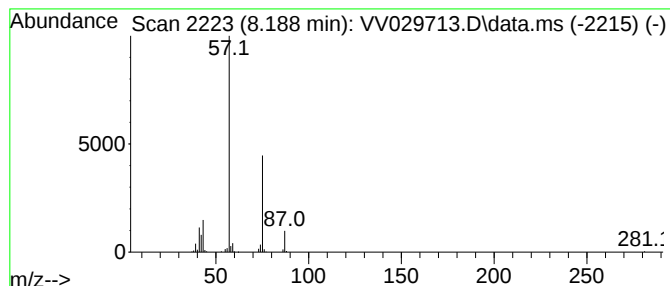
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.188	4.85 ug/L	123992	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	53
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029713.D
Acq On : 19 Dec 2022 11:55
Operator : SY/MD
Sample : N6075-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM1

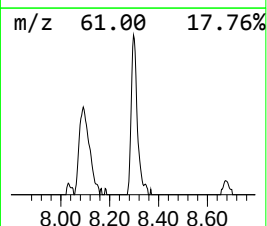
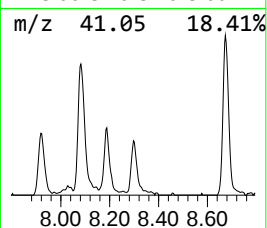
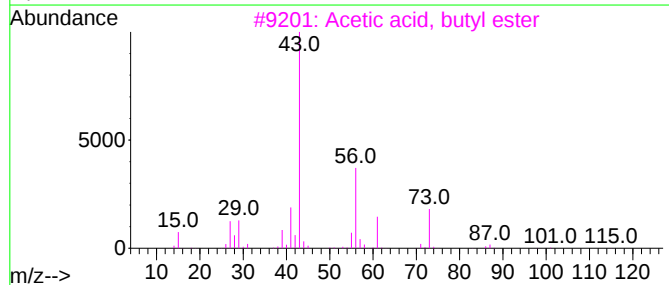
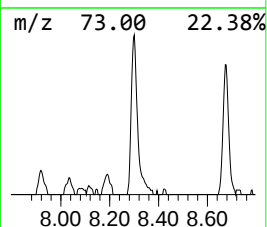
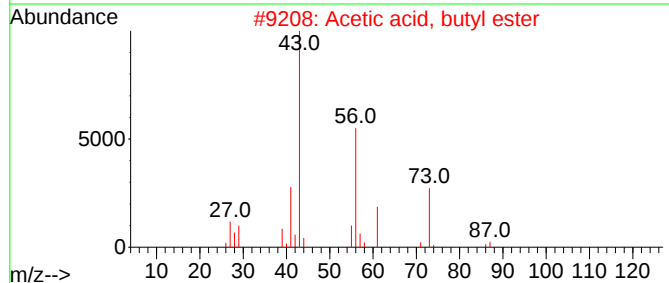
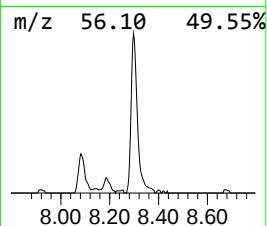
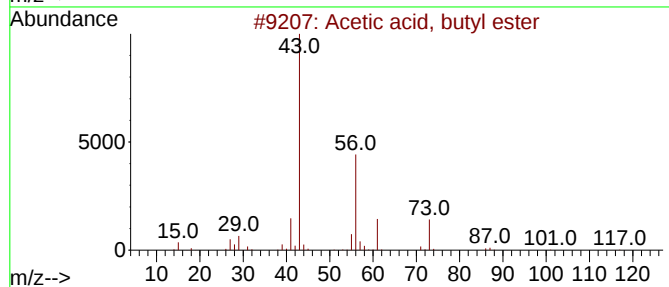
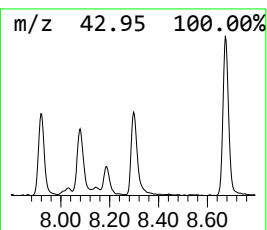
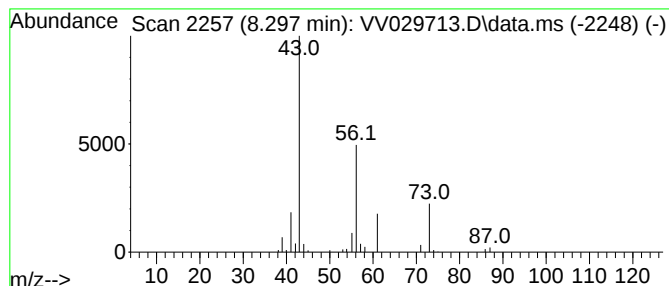
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.297	3.01 ug/L	77069	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	64
4	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	42
5	Acetic acid, hexyl ester			144	C8H16O2	000142-92-7	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029713.D
Acq On : 19 Dec 2022 11:55
Operator : SY/MD
Sample : N6075-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM1

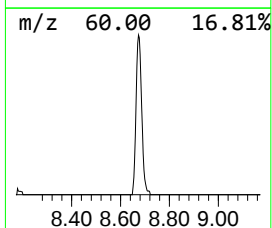
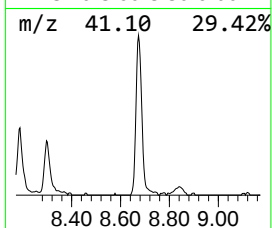
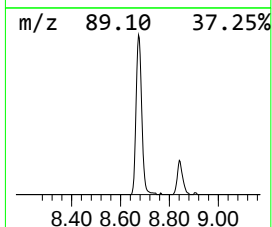
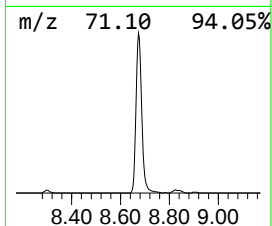
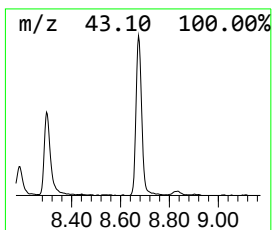
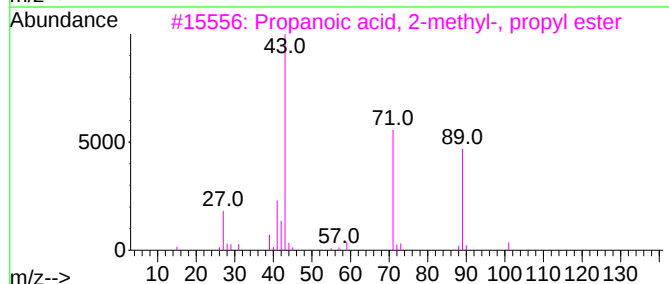
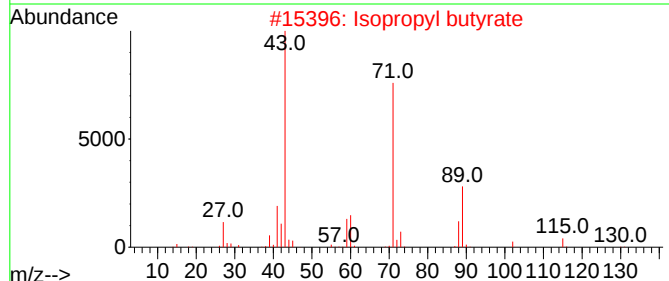
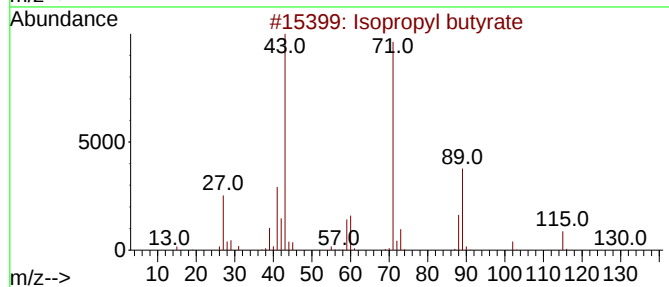
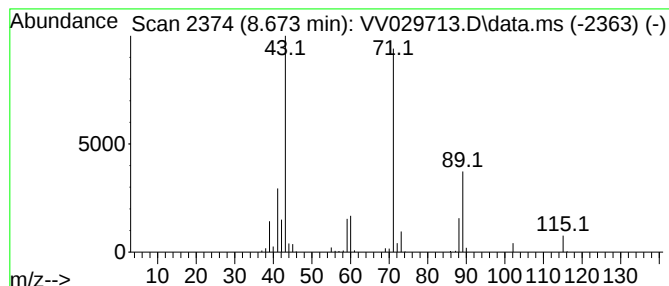
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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.
8.673	8.31 ug/L	212443	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			Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	72
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5			Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW121922\
Data File : VV029713.D
Acq On : 19 Dec 2022 11:55
Operator : SY/MD
Sample : N6075-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM1

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	6.458	13.7	ug/L	289519	1	5.609	1060860	50.0
Propanoic acid,...	7.182	2.8	ug/L	60005	1	5.609	1060860	50.0
Propanoic acid,...	7.921	2.9	ug/L	73839	2	8.844	1278990	50.0
Propanoic acid,...	8.188	4.8	ug/L	123992	2	8.844	1278990	50.0
Acetic acid, bu...	8.297	3.0	ug/L	77069	2	8.844	1278990	50.0
Isopropyl butyrate	8.673	8.3	ug/L	212443	2	8.844	1278990	50.0