

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
 Data File : VV033565.D
 Acq On : 10 Jan 2024 17:06
 Operator : SY/MD
 Sample : P1016-05 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMH5

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\SFAMVLM011024WMA.M
 Title : VOC Analysis

Signal : TIC: VV033565.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.162	34	38	44	rBV	2438	2527	0.19%	0.023%
2	1.220	50	56	58	rBV4	2931	3129	0.24%	0.029%
3	1.278	68	74	88	rBV	190817	199630	15.17%	1.823%
4	1.529	145	152	171	rVB	145004	178371	13.55%	1.629%
5	2.060	307	317	329	rBV	293872	431720	32.81%	3.943%
6	2.323	396	399	404	rBV7	769	662	0.05%	0.006%
7	2.449	430	438	447	rBV	6679	10684	0.81%	0.098%
8	2.555	467	471	472	rVV3	823	679	0.05%	0.006%
9	2.609	486	488	492	rVB4	519	320	0.02%	0.003%
10	2.892	573	576	583	rBV7	599	650	0.05%	0.006%
11	2.995	606	608	612	rVB3	664	362	0.03%	0.003%
12	3.105	630	642	656	rBV3	7626	19445	1.48%	0.178%
13	3.333	711	713	717	rVB3	556	336	0.03%	0.003%
14	3.365	717	723	728	rBV9	598	640	0.05%	0.006%
15	3.420	736	740	745	rVB6	649	568	0.04%	0.005%
16	3.445	745	748	751	rBV3	523	317	0.02%	0.003%
17	3.523	769	772	775	rVB3	709	408	0.03%	0.004%
18	3.648	809	811	815	rBV3	381	354	0.03%	0.003%
19	3.783	845	853	896	rBV	90940	255519	19.42%	2.334%
20	4.249	981	998	1026	rVV	192889	500597	38.04%	4.572%
21	4.465	1063	1065	1072	rVB6	668	642	0.05%	0.006%
22	4.567	1095	1097	1100	rBV4	521	332	0.03%	0.003%
23	4.680	1128	1132	1136	rVB5	397	353	0.03%	0.003%
24	4.712	1140	1142	1146	rBV3	429	366	0.03%	0.003%
25	4.850	1182	1185	1190	rVB4	571	537	0.04%	0.005%
26	4.876	1190	1193	1196	rBV4	595	466	0.04%	0.004%
27	4.957	1201	1218	1254	rBV2	492686	1315976	100.00%	12.019%
28	5.214	1289	1298	1319	rBV3	8062	20527	1.56%	0.187%
29	5.535	1385	1398	1430	rBV	402526	836566	63.57%	7.640%
30	5.728	1456	1458	1462	rBV5	559	342	0.03%	0.003%
31	5.831	1480	1490	1505	rBV5	5578	12159	0.92%	0.111%
32	5.924	1515	1519	1522	rVB4	824	594	0.05%	0.005%
33	5.989	1522	1539	1574	rBV	287532	607159	46.14%	5.545%
34	6.310	1627	1639	1644	rBV4	2356	5471	0.42%	0.050%
35	6.394	1656	1665	1705	rBV	108291	222215	16.89%	2.029%
36	6.812	1791	1795	1797	rBV3	490	404	0.03%	0.004%

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 Title : VOC Analysis

37	6.841	1800	1804	1806	rBV6	537	322	0.02%	0.003%
38	6.915	1810	1827	1855	rBV	172324	326756	24.83%	2.984%
39	7.124	1883	1892	1904	rBV2	26732	46491	3.53%	0.425%
40	7.243	1918	1929	1953	rBV	593527	1047427	79.59%	9.566%
41	7.555	2015	2026	2047	rBV	147797	273018	20.75%	2.493%
42	7.773	2091	2094	2098	rVB6	653	419	0.03%	0.004%
43	7.863	2111	2122	2141	rBV	39475	69910	5.31%	0.638%
44	7.976	2148	2157	2162	rBV4	7810	11609	0.88%	0.106%
45	8.024	2163	2172	2198	rVV	340984	642465	48.82%	5.868%
46	8.130	2199	2205	2231	rVV	55362	108518	8.25%	0.991%
47	8.246	2234	2241	2272	rVB2	29629	61380	4.66%	0.561%
48	8.548	2330	2335	2340	rVB6	546	505	0.04%	0.005%
49	8.619	2344	2357	2383	rBV	109619	181728	13.81%	1.660%
50	8.786	2396	2409	2437	rBV	609139	1014602	77.10%	9.266%
51	9.027	2479	2484	2488	rVB4	979	978	0.07%	0.009%
52	9.059	2488	2494	2498	rBV6	1395	2095	0.16%	0.019%
53	9.153	2519	2523	2524	rBV3	445	330	0.03%	0.003%
54	9.349	2577	2584	2586	rBV3	1043	1097	0.08%	0.010%
55	9.500	2621	2631	2641	rBV2	6160	12039	0.91%	0.110%
56	9.612	2663	2666	2669	rBV3	629	344	0.03%	0.003%
57	9.635	2669	2673	2676	rBV5	400	324	0.02%	0.003%
58	9.780	2715	2718	2721	rBV3	427	319	0.02%	0.003%
59	9.876	2746	2748	2751	rVV3	490	318	0.02%	0.003%
60	10.107	2815	2820	2821	rBV3	874	599	0.05%	0.005%
61	10.152	2821	2834	2859	rVB	361993	566514	43.05%	5.174%
62	10.378	2900	2904	2906	rBV3	640	381	0.03%	0.003%
63	10.445	2923	2925	2929	rBV3	328	333	0.03%	0.003%
64	10.529	2946	2951	2952	rBV4	429	317	0.02%	0.003%
65	10.779	3023	3029	3033	rBV4	518	483	0.04%	0.004%
66	10.802	3034	3036	3043	rVB3	454	380	0.03%	0.003%
67	10.847	3047	3050	3051	rBV	579	324	0.02%	0.003%
68	11.011	3096	3101	3105	rVB4	466	409	0.03%	0.004%
69	11.185	3144	3155	3180	rBV	628802	981434	74.58%	8.963%
70	11.493	3248	3251	3257	rVB5	555	469	0.04%	0.004%
71	11.561	3257	3272	3297	rBV	586501	928312	70.54%	8.478%
72	11.779	3337	3340	3343	rBV3	479	330	0.03%	0.003%
73	11.844	3355	3360	3362	rBV3	519	405	0.03%	0.004%
74	11.963	3394	3397	3400	rVV2	727	530	0.04%	0.005%
75	12.146	3452	3454	3460	rVB4	420	364	0.03%	0.003%
76	12.332	3508	3512	3513	rBV2	604	368	0.03%	0.003%

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 Title : VOC Analysis

77	12.365	3518	3522	3525	rBV4	654	439	0.03%	0.004%
78	12.435	3539	3544	3546	rBV3	838	704	0.05%	0.006%
79	12.522	3562	3571	3575	rBV7	581	931	0.07%	0.009%
80	12.593	3589	3593	3600	rBV6	615	790	0.06%	0.007%
81	12.657	3609	3613	3615	rBV3	394	340	0.03%	0.003%
82	12.808	3655	3660	3662	rBV5	571	421	0.03%	0.004%
83	12.834	3666	3668	3674	rVV4	464	400	0.03%	0.004%
84	12.924	3692	3696	3700	rVB3	550	506	0.04%	0.005%
85	12.950	3700	3704	3706	rBV3	577	447	0.03%	0.004%
86	13.049	3732	3735	3737	rBV2	588	358	0.03%	0.003%
87	13.162	3768	3770	3774	rVB3	531	356	0.03%	0.003%
88	13.207	3777	3784	3794	rBV7	2814	4391	0.33%	0.040%
89	13.374	3833	3836	3844	rVB7	598	744	0.06%	0.007%
90	13.451	3852	3860	3872	rVB2	8401	13754	1.05%	0.126%
91	13.683	3923	3932	3939	rBV7	1824	2738	0.21%	0.025%
92	13.805	3965	3970	3972	rBV2	647	505	0.04%	0.005%
93	13.847	3980	3983	3987	rVB3	651	500	0.04%	0.005%
94	14.127	4068	4070	4074	rVB3	917	498	0.04%	0.005%
95	14.156	4074	4079	4082	rBV5	674	632	0.05%	0.006%
96	14.262	4109	4112	4116	rVV5	447	415	0.03%	0.004%
97	14.345	4134	4138	4143	rBV6	721	773	0.06%	0.007%
98	14.512	4184	4190	4198	rBV8	566	970	0.07%	0.009%
99	14.606	4216	4219	4220	rBV4	538	347	0.03%	0.003%
100	14.844	4286	4293	4297	rBV7	888	1341	0.10%	0.012%

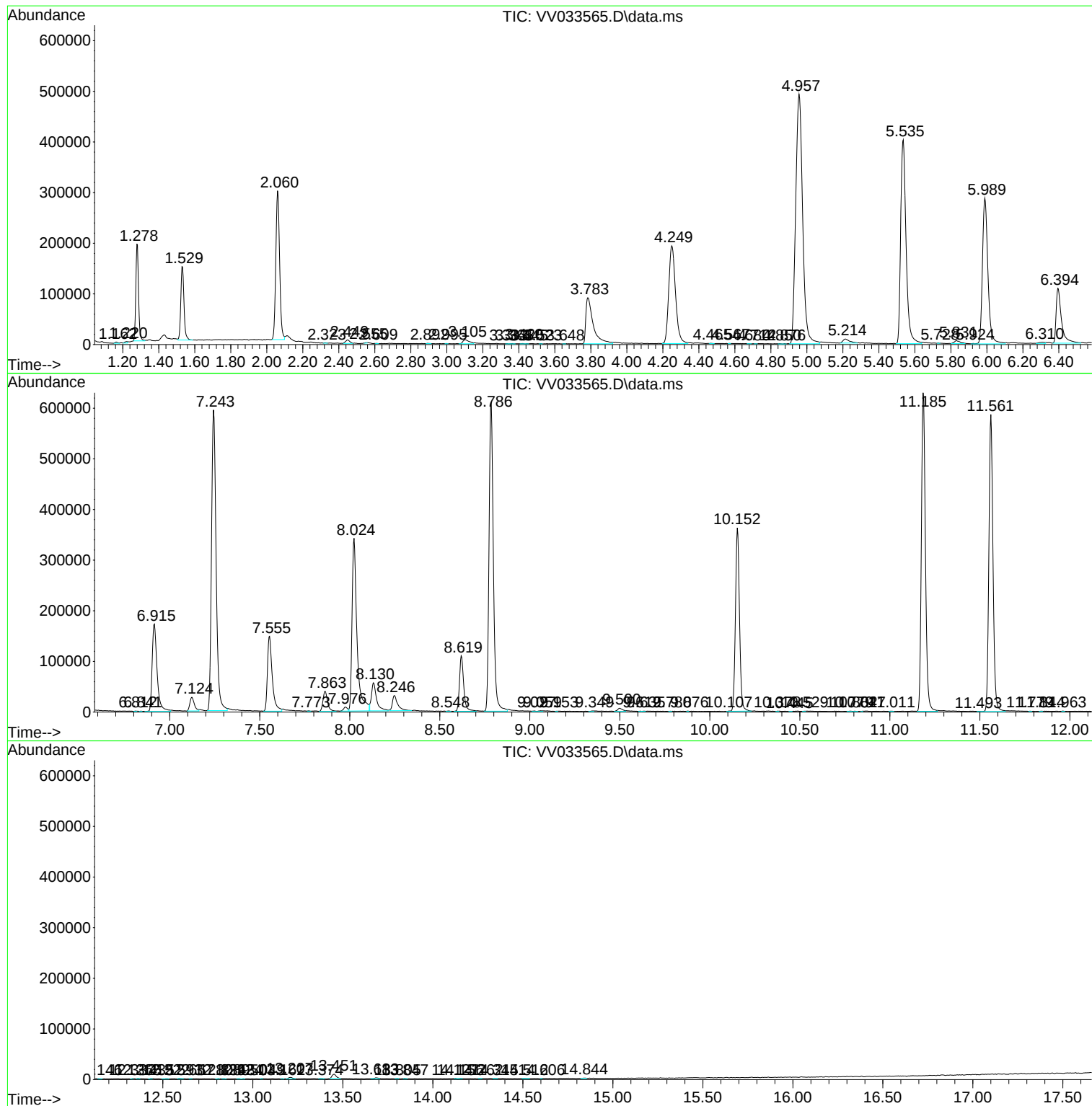
Sum of corrected areas: 10949273

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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



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ClientSampleId :
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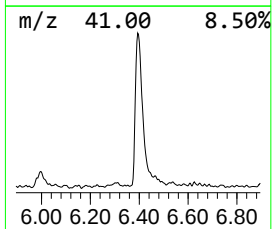
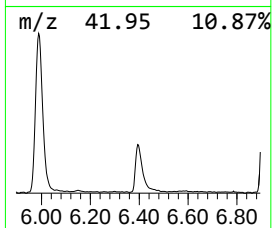
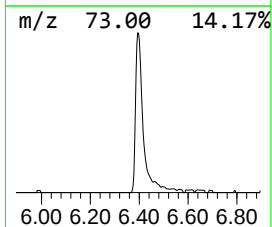
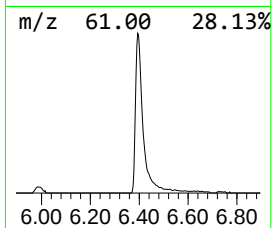
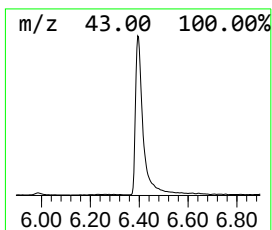
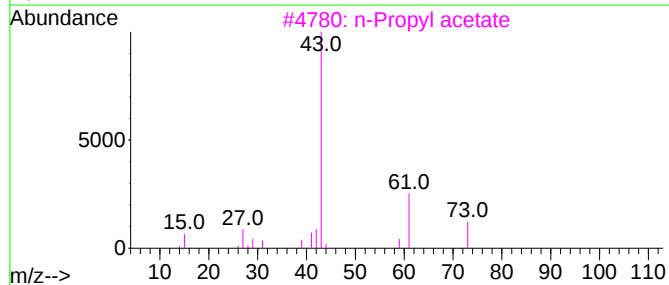
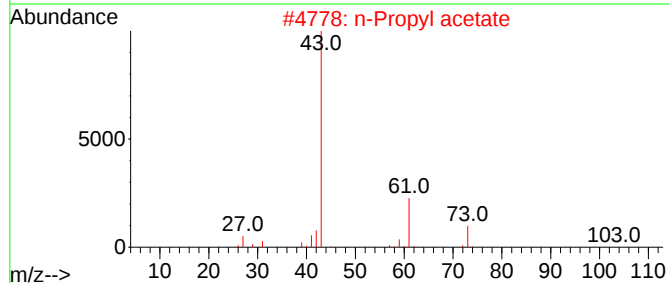
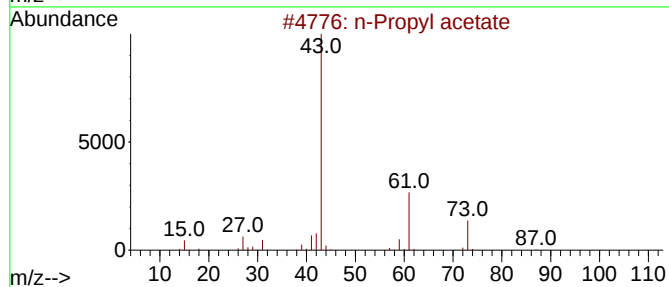
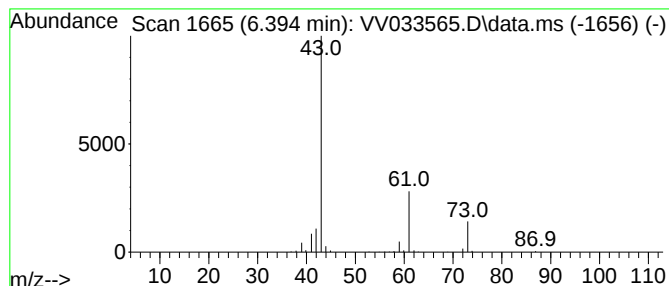
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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.
6.394	13.28 ug/L	222215	1,4-Difluorobenzene	5.535

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	Isopropyl acetate			102	C5H10O2	000108-21-4	38



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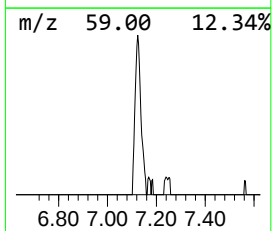
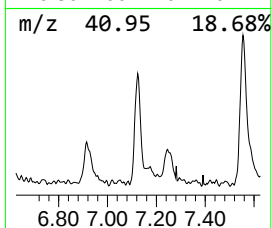
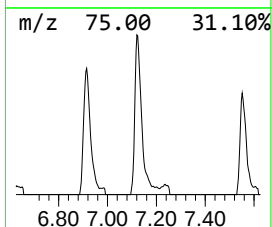
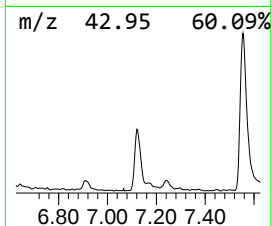
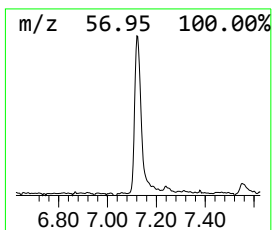
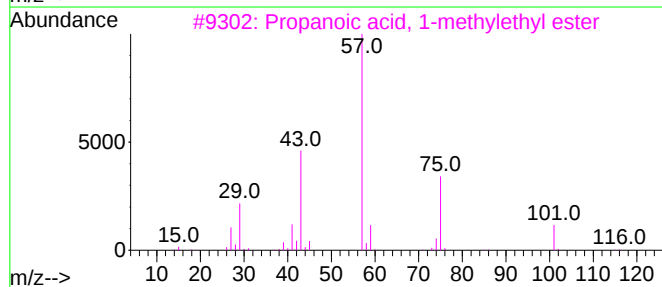
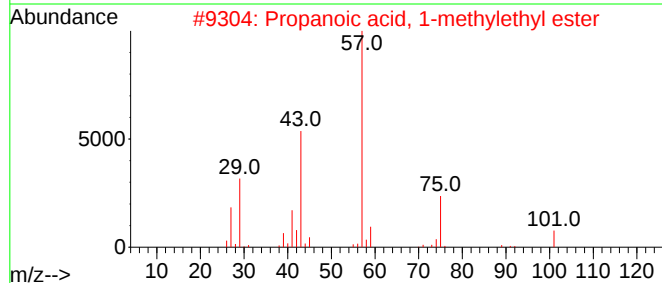
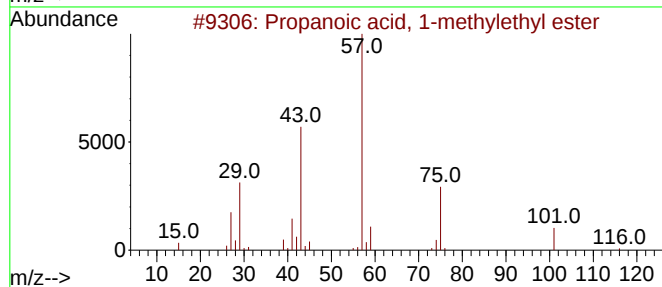
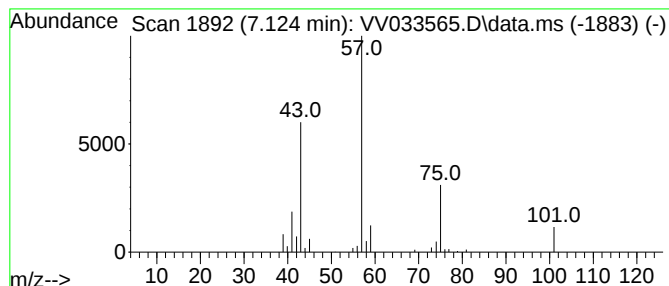
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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.
7.124	2.78 ug/L	46491	1,4-Difluorobenzene	5.535

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	78
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40



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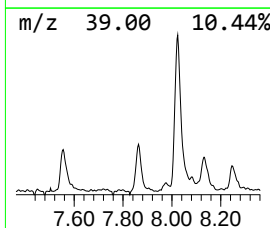
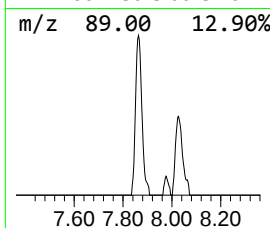
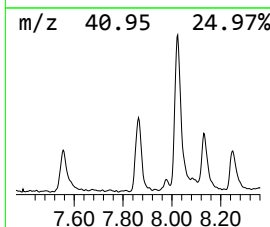
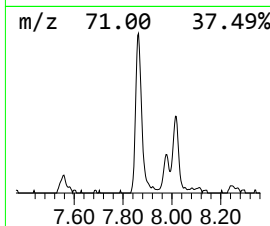
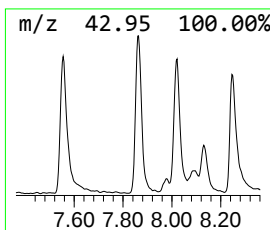
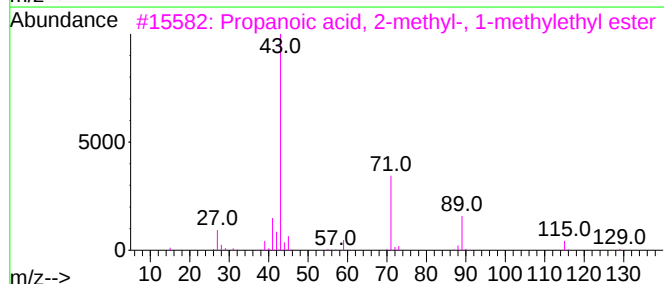
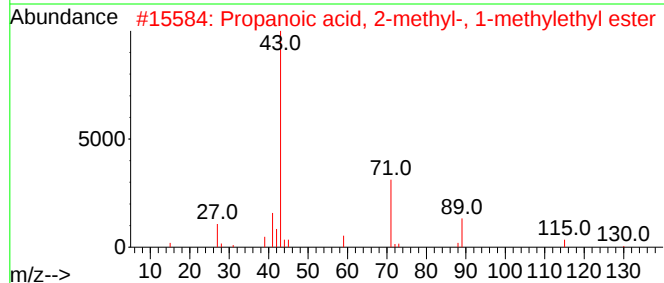
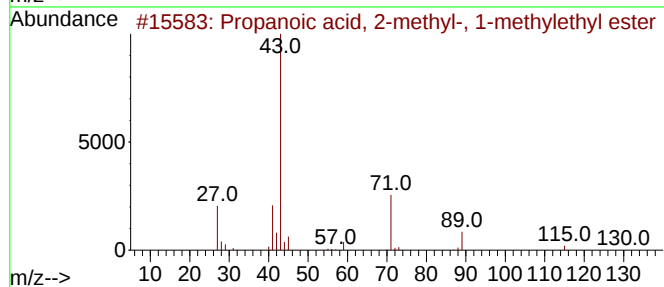
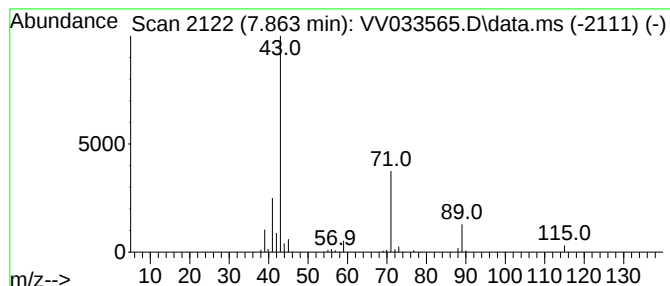
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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.
7.863	3.45 ug/L	69910	Chlorobenzene-d5	8.786

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-, 1-met...	130	C7H14O2	000617-50-5	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033565.D
Acq On : 10 Jan 2024 17:06
Operator : SY/MD
Sample : P1016-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMH5

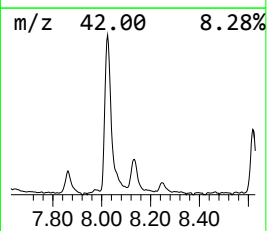
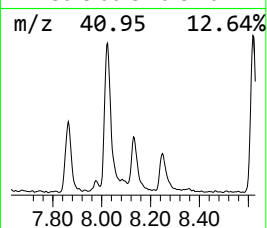
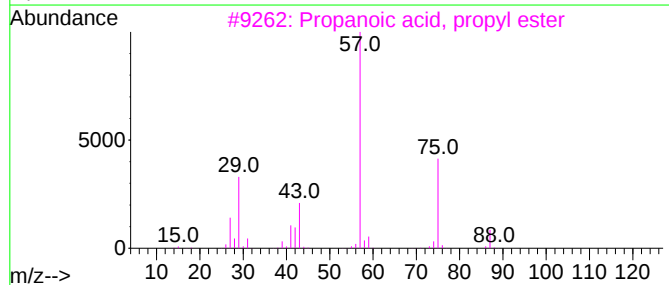
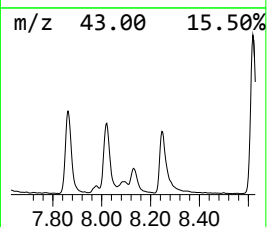
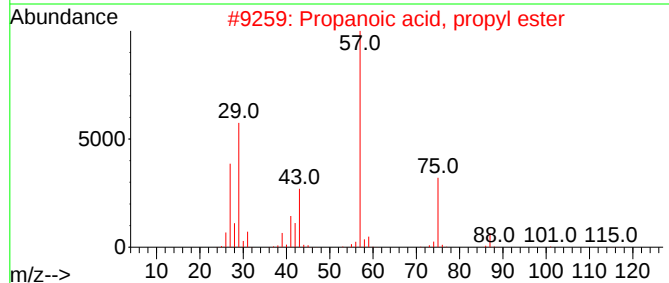
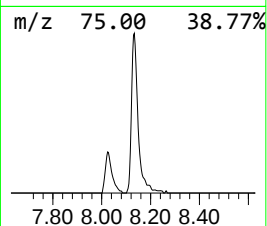
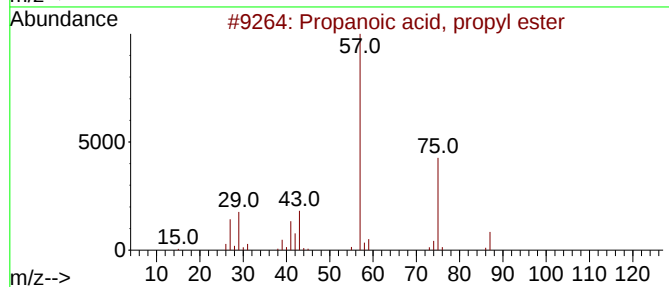
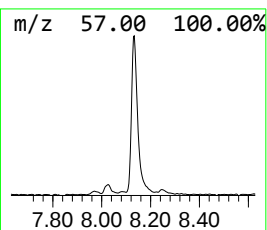
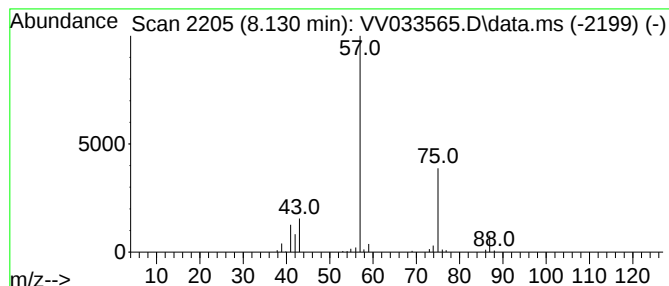
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Quant Title : VOC Analysis

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.
8.130	5.35 ug/L	108518	Chlorobenzene-d5	8.786

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	78
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033565.D
Acq On : 10 Jan 2024 17:06
Operator : SY/MD
Sample : P1016-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMH5

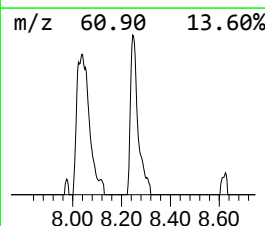
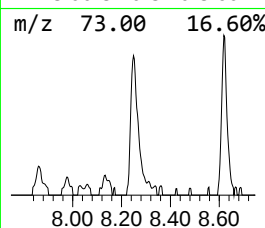
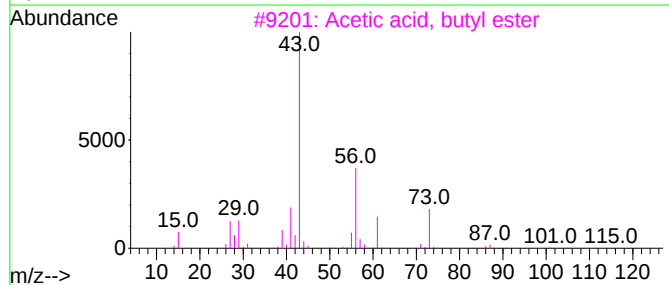
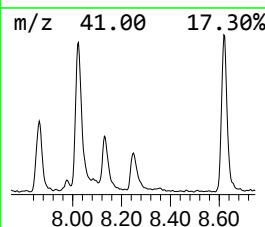
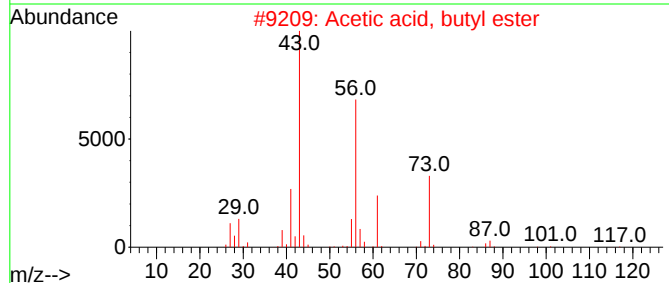
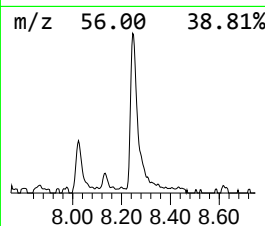
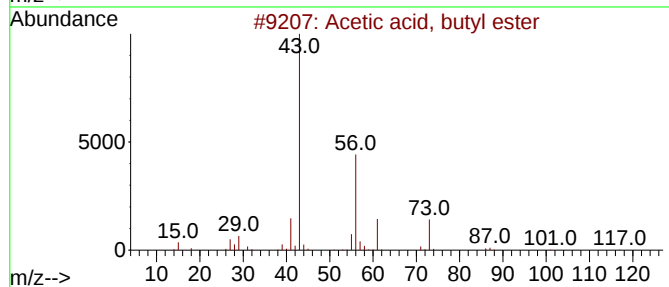
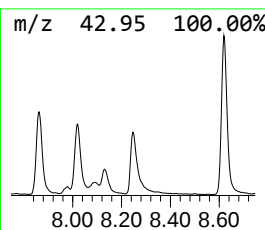
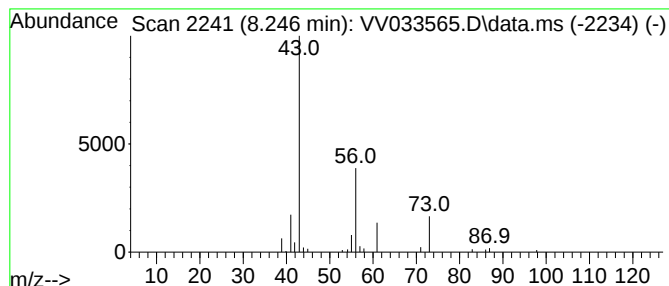
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Quant Title : VOC Analysis

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.
8.246	3.02 ug/L	61380	Chlorobenzene-d5	8.786

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	56
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
5			Isobutylamine	73	C4H11N	000078-81-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033565.D
Acq On : 10 Jan 2024 17:06
Operator : SY/MD
Sample : P1016-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMH5

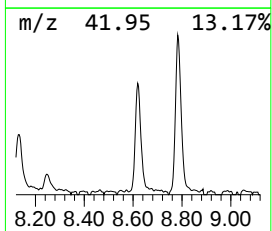
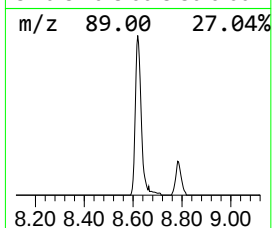
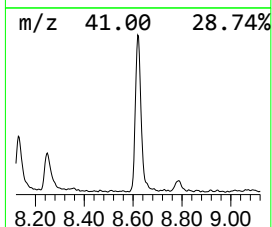
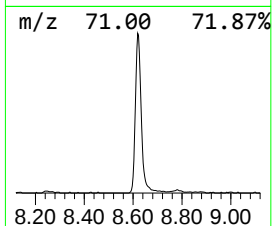
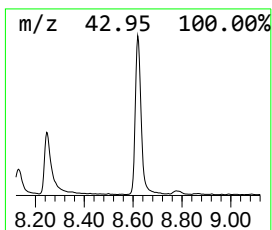
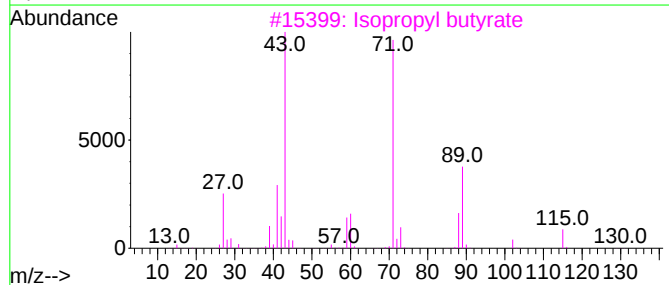
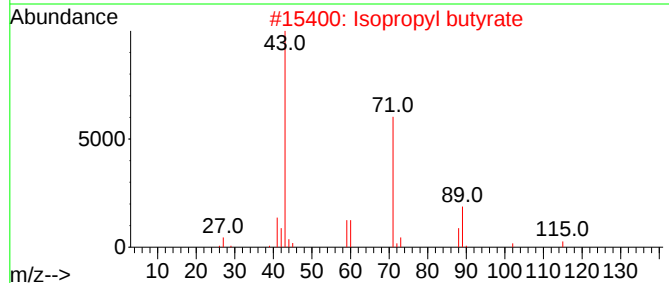
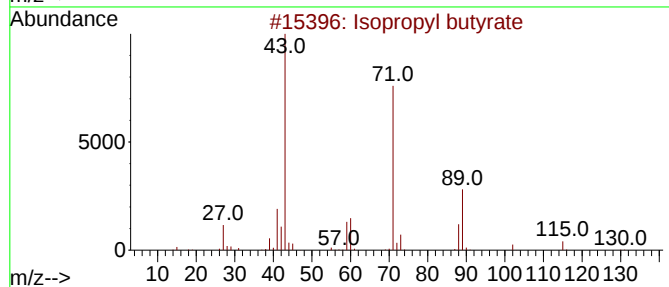
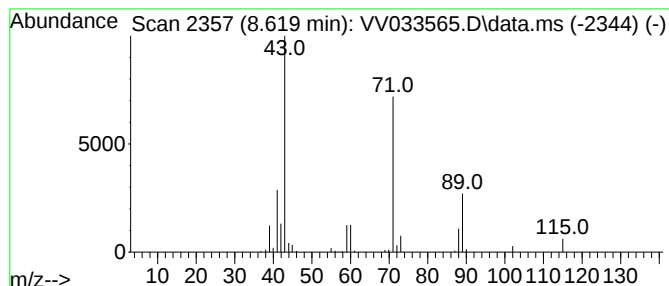
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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.
8.619	8.96 ug/L	181728	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	86
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033565.D
Acq On : 10 Jan 2024 17:06
Operator : SY/MD
Sample : P1016-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMH5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.394	13.3	ug/L	222215	1	5.535	836566	50.0
Propanoic acid,...	7.124	2.8	ug/L	46491	1	5.535	836566	50.0
Propanoic acid,...	7.863	3.5	ug/L	69910	2	8.786	1014600	50.0
Propanoic acid,...	8.130	5.3	ug/L	108518	2	8.786	1014600	50.0
Acetic acid, bu...	8.246	3.0	ug/L	61380	2	8.786	1014600	50.0
Isopropyl butyrate	8.619	9.0	ug/L	181728	2	8.786	1014600	50.0