

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122123\
 Data File : VV033530.D
 Acq On : 21 Dec 2023 13:28
 Operator : SY/MD
 Sample : PB157957TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB957

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\SFAMVLM121523WMA.M
 Title : VOC Analysis

Signal : TIC: VV033530.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.281	68	75	90	rBV	131336	135105	13.64%	1.590%
2	1.532	146	153	164	rVB	117941	140894	14.22%	1.658%
3	2.063	309	318	329	rBV	225592	327630	33.07%	3.856%
4	2.625	489	493	496	rBV5	1648	1337	0.13%	0.016%
5	2.658	501	503	504	rBV2	900	393	0.04%	0.005%
6	2.693	510	514	516	rBV4	1622	1168	0.12%	0.014%
7	2.828	554	556	561	rBV6	1354	1001	0.10%	0.012%
8	2.863	564	567	572	rBV6	1096	959	0.10%	0.011%
9	3.011	611	613	614	rBV	1038	396	0.04%	0.005%
10	3.227	677	680	684	rBV5	1280	702	0.07%	0.008%
11	3.301	701	703	708	rVB6	1378	905	0.09%	0.011%
12	3.339	713	715	716	rBV2	640	352	0.04%	0.004%
13	3.455	748	751	752	rBV3	870	467	0.05%	0.005%
14	3.558	781	783	787	rBV5	1385	983	0.10%	0.012%
15	3.632	805	806	807	rBV2	689	252	0.03%	0.003%
16	3.703	826	828	829	rBV2	885	223	0.02%	0.003%
17	3.783	845	853	876	rBV	53645	149915	15.13%	1.764%
18	4.143	961	965	968	rVB5	1931	1470	0.15%	0.017%
19	4.249	985	998	1025	rVB	160585	408305	41.22%	4.805%
20	4.539	1087	1088	1096	rVB6	1536	1005	0.10%	0.012%
21	4.603	1105	1108	1110	rBV4	1304	846	0.09%	0.010%
22	4.680	1130	1132	1133	rBV2	1157	444	0.04%	0.005%
23	4.818	1172	1175	1179	rBV5	1884	1808	0.18%	0.021%
24	4.876	1190	1193	1194	rBV3	759	313	0.03%	0.004%
25	4.957	1202	1218	1249	rBV2	369354	990620	100.00%	11.658%
26	5.394	1352	1354	1355	rBV3	1545	538	0.05%	0.006%
27	5.535	1386	1398	1429	rBV	286974	607784	61.35%	7.153%
28	5.915	1514	1516	1517	rBV2	1045	400	0.04%	0.005%
29	5.937	1521	1523	1524	rBV2	1190	550	0.06%	0.006%
30	5.989	1527	1539	1565	rVV2	221418	465857	47.03%	5.482%
31	6.391	1655	1664	1697	rBV	173371	342906	34.62%	4.035%
32	6.915	1817	1827	1845	rBV	110865	210036	21.20%	2.472%
33	7.120	1883	1891	1905	rBV	42465	69915	7.06%	0.823%
34	7.243	1919	1929	1948	rBV	420180	737745	74.47%	8.682%
35	7.551	2016	2025	2046	rBV2	127055	241363	24.36%	2.840%
36	7.860	2111	2121	2137	rBV2	67126	117499	11.86%	1.383%

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Integrator: RTE

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 Title : VOC Analysis

37	8.024	2164	2172	2196	rBV2	204452	385653	38.93%	4.538%
38	8.243	2233	2240	2260	rVB	52132	89520	9.04%	1.053%
39	8.619	2347	2357	2380	rBV	187050	315933	31.89%	3.718%
40	8.783	2398	2408	2430	rBV	512919	855411	86.35%	10.067%
41	9.304	2568	2570	2571	rBV2	1119	464	0.05%	0.005%
42	9.464	2619	2620	2621	rBV2	911	248	0.03%	0.003%
43	9.493	2621	2629	2639	rVV4	10366	18982	1.92%	0.223%
44	9.873	2741	2747	2751	rBV9	1440	1698	0.17%	0.020%
45	9.889	2751	2752	2753	rBV2	604	178	0.02%	0.002%
46	9.898	2753	2755	2756	rBV2	1029	295	0.03%	0.003%
47	10.008	2787	2789	2790	rBV2	870	324	0.03%	0.004%
48	10.152	2823	2834	2854	rBV	301144	468411	47.28%	5.512%
49	10.278	2872	2873	2874	rBV	1231	417	0.04%	0.005%
50	10.374	2899	2903	2906	rBV4	1691	1614	0.16%	0.019%
51	10.596	2970	2972	2977	rBV4	662	577	0.06%	0.007%
52	10.648	2986	2988	2990	rBV3	1060	744	0.08%	0.009%
53	10.776	3025	3028	3031	rBV5	1318	1063	0.11%	0.013%
54	10.924	3072	3074	3078	rVB4	1200	609	0.06%	0.007%
55	10.943	3078	3080	3083	rBV3	1179	813	0.08%	0.010%
56	11.185	3145	3155	3178	rBV	435214	681394	68.78%	8.019%
57	11.509	3255	3256	3257	rBV	869	300	0.03%	0.004%
58	11.561	3261	3272	3293	rVV	431868	693675	70.02%	8.163%
59	11.828	3353	3355	3358	rBV4	995	516	0.05%	0.006%
60	11.924	3383	3385	3390	rBV5	1049	777	0.08%	0.009%
61	12.123	3443	3447	3449	rBV4	1337	947	0.10%	0.011%
62	12.185	3463	3466	3468	rBV3	1009	726	0.07%	0.009%
63	12.480	3551	3558	3562	rBV7	1927	2037	0.21%	0.024%
64	12.513	3562	3568	3569	rBV4	1072	1072	0.11%	0.013%
65	12.625	3600	3603	3607	rBV5	862	686	0.07%	0.008%
66	12.818	3661	3663	3666	rBV3	1005	640	0.06%	0.008%
67	12.869	3677	3679	3680	rBV2	871	388	0.04%	0.005%
68	12.972	3710	3711	3712	rBV	681	230	0.02%	0.003%
69	13.143	3762	3764	3766	rBV3	748	395	0.04%	0.005%
70	13.352	3827	3829	3833	rBV5	1191	1065	0.11%	0.013%
71	13.651	3916	3922	3924	rBV5	1638	1624	0.16%	0.019%
72	14.120	4066	4068	4072	rBV4	881	452	0.05%	0.005%
73	14.236	4101	4104	4107	rBV4	1723	775	0.08%	0.009%
74	14.310	4125	4127	4129	rBV3	1149	599	0.06%	0.007%
75	14.336	4133	4135	4137	rBV3	1078	487	0.05%	0.006%
76	14.365	4141	4144	4147	rBV5	1123	937	0.09%	0.011%

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Title : VOC Analysis

77	14.403	4154	4156	4157	rBV2	874	251	0.03%	0.003%
78	14.500	4184	4186	4189	rVB4	1646	681	0.07%	0.008%
79	14.545	4198	4200	4201	rBV2	793	289	0.03%	0.003%
80	14.641	4228	4230	4232	rBV3	978	488	0.05%	0.006%
81	14.770	4269	4270	4273	rBV2	968	390	0.04%	0.005%
82	15.500	4495	4497	4499	rBV2	958	529	0.05%	0.006%

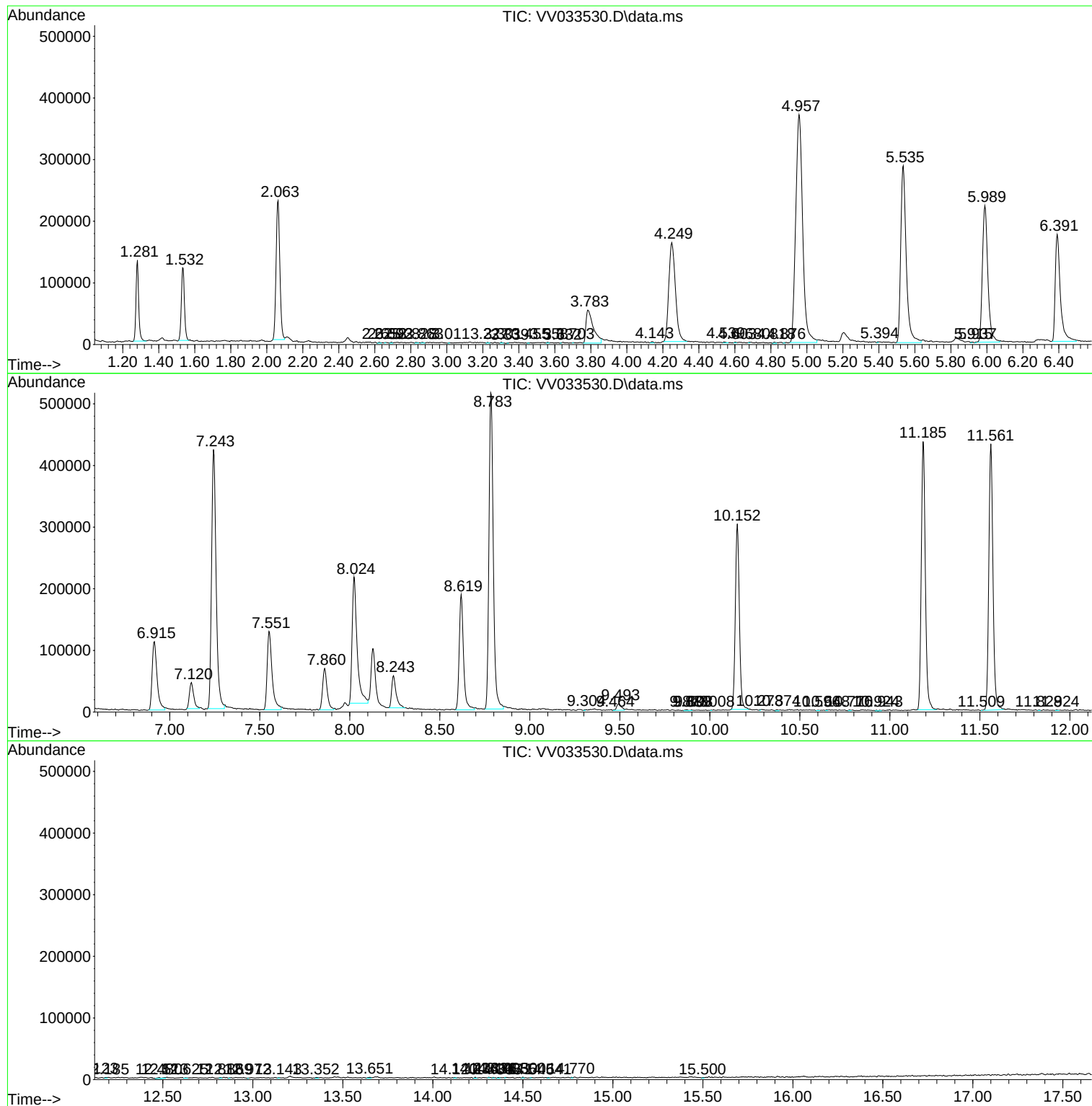
Sum of corrected areas: 8497390

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM121523WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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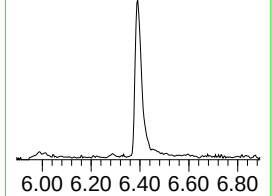
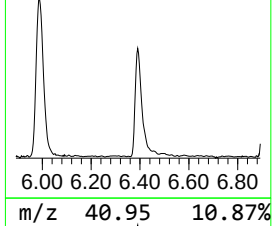
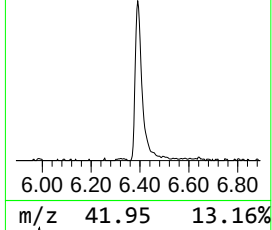
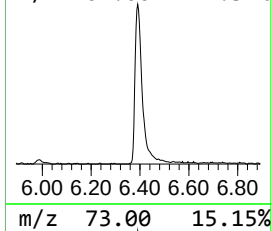
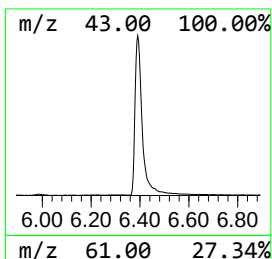
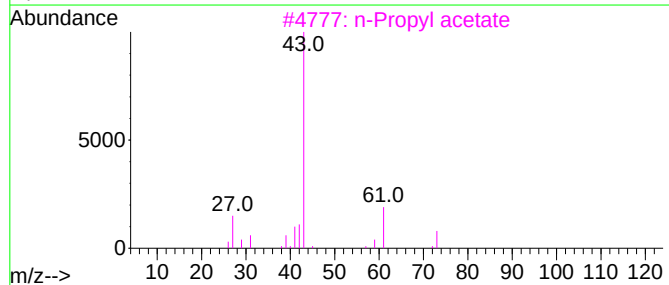
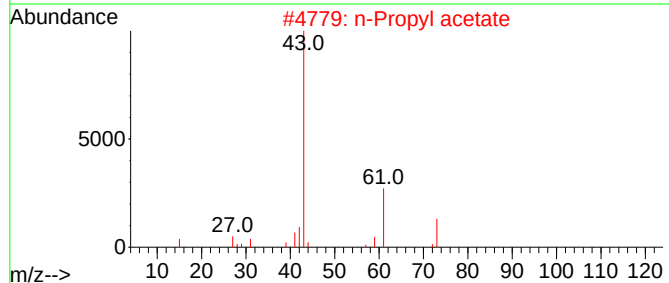
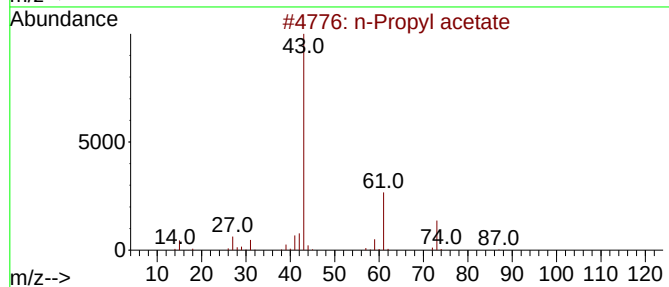
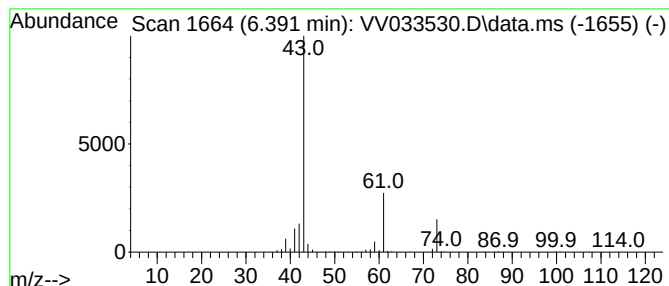
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM121523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.391	28.21 ug/L	342906	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	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	40



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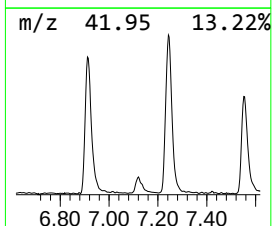
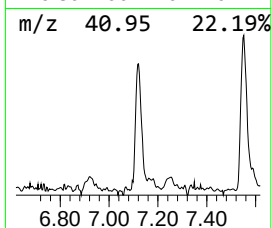
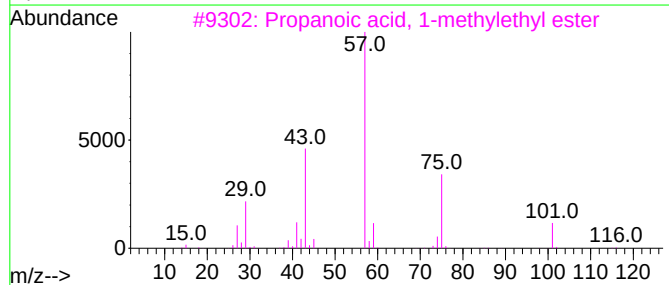
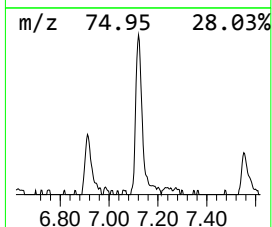
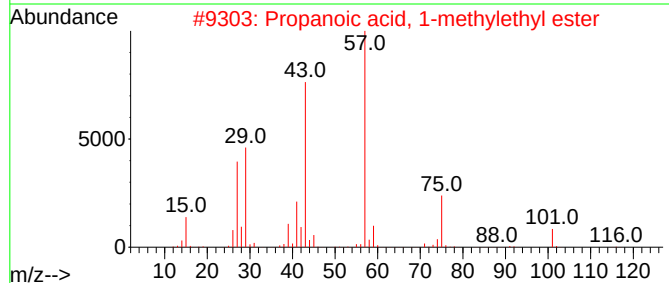
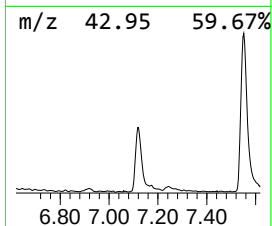
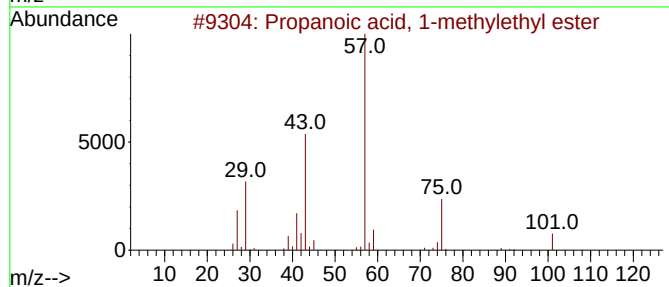
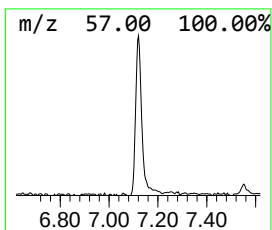
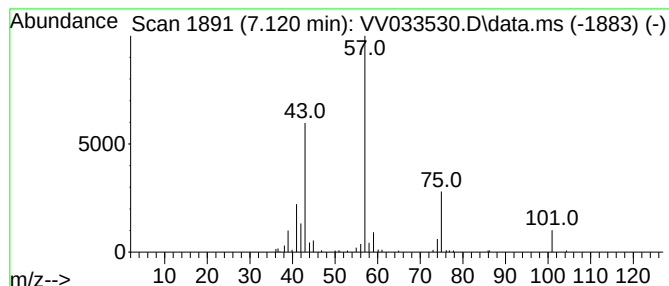
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.120	5.75 ug/L	69915	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	78
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50



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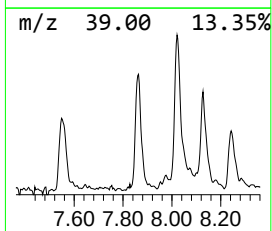
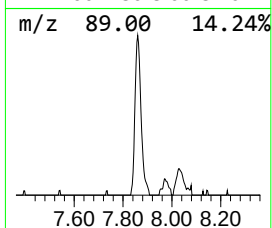
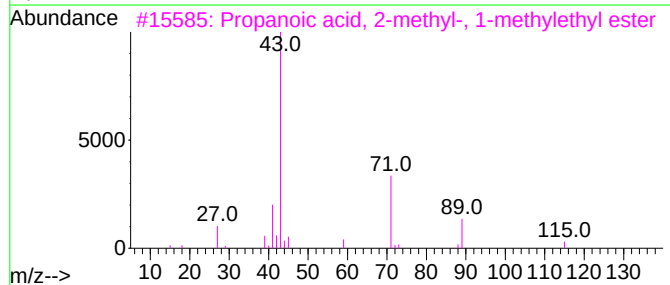
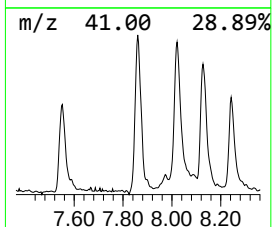
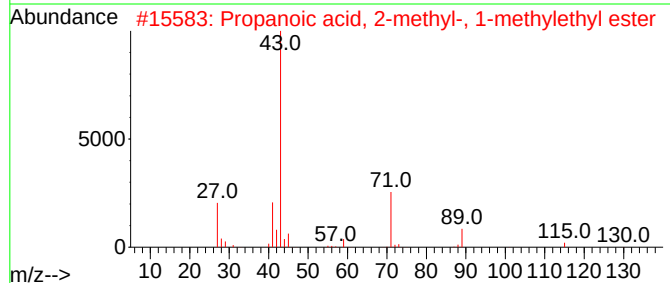
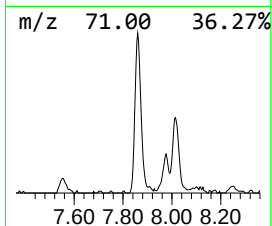
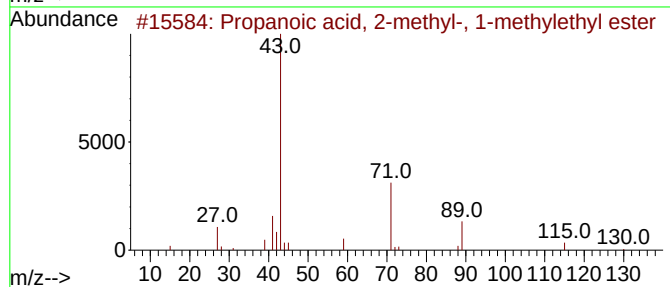
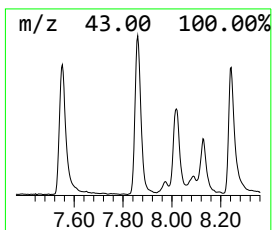
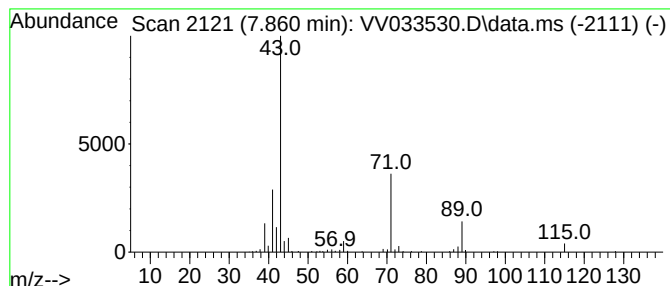
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.860	6.87 ug/L	117499	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	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-, propy...	130	C7H14O2	000644-49-5	72



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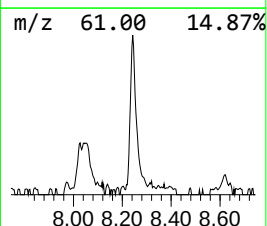
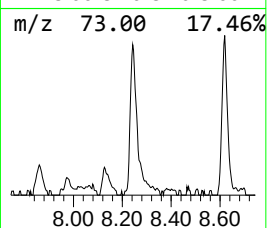
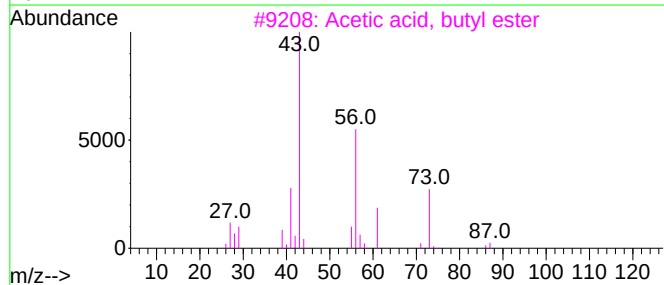
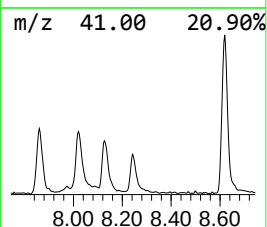
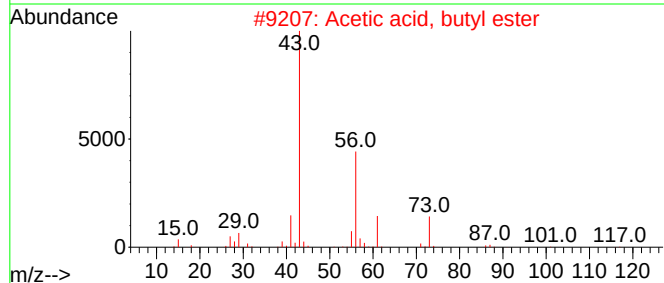
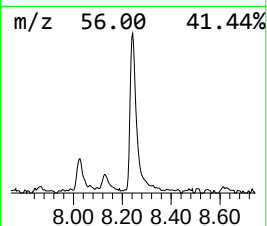
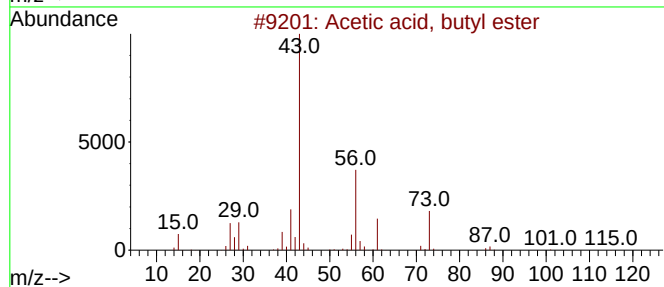
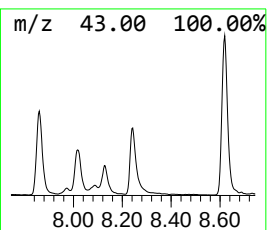
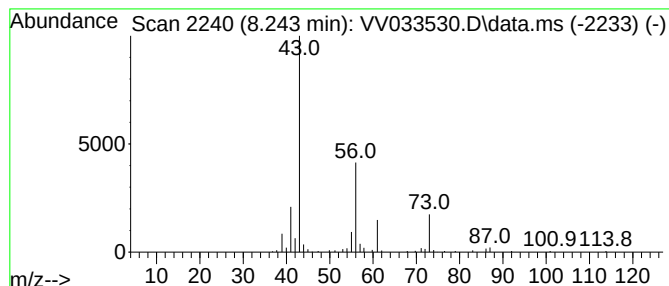
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Quant Title : VOC Analysis

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

Peak Number 5 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.243	5.23 ug/L	89520	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	78
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
5			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122123\
Data File : VV033530.D
Acq On : 21 Dec 2023 13:28
Operator : SY/MD
Sample : PB157957TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB957

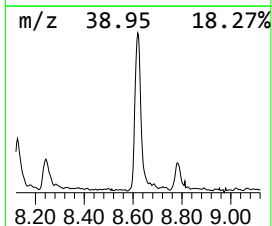
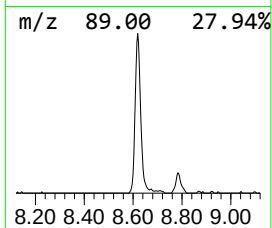
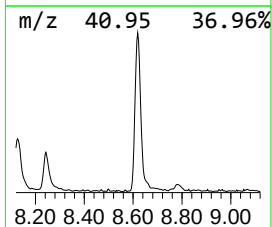
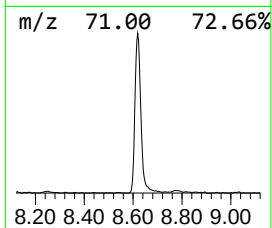
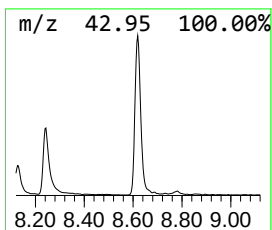
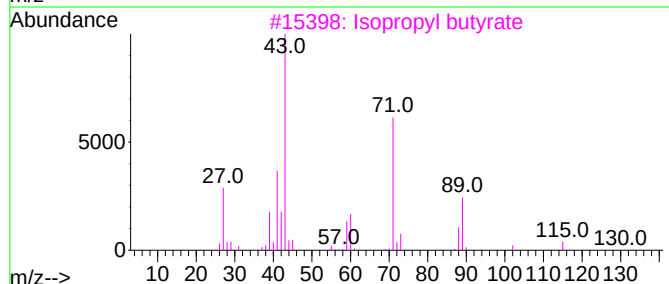
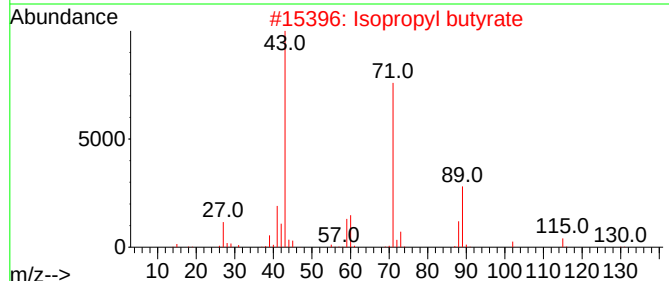
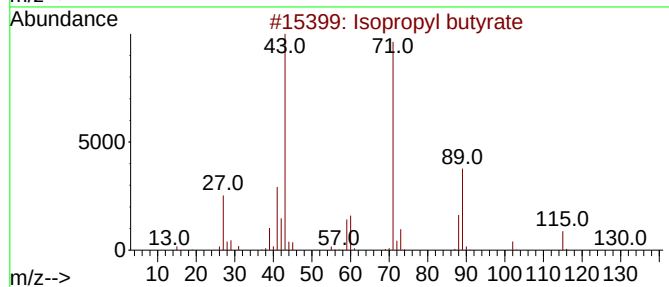
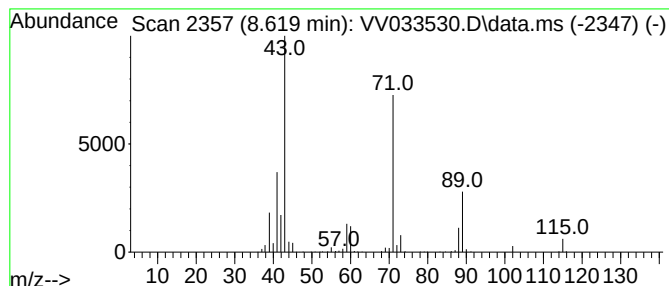
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Quant Title : VOC Analysis

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

Peak Number 6 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	18.47 ug/L	315933	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		Isopropyl butyrate	130	C7H14O2	000638-11-9	83
5		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW122123\
Data File : VV033530.D
Acq On : 21 Dec 2023 13:28
Operator : SY/MD
Sample : PB157957TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB957

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM121523WMA.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	6.391	28.2	ug/L	342906	1	5.535	607784	50.0
Propanoic acid,...	7.120	5.8	ug/L	69915	1	5.535	607784	50.0
Propanoic acid,...	7.860	6.9	ug/L	117499	2	8.786	855411	50.0
Acetic acid, bu...	8.243	5.2	ug/L	89520	2	8.786	855411	50.0
Isopropyl butyrate	8.619	18.5	ug/L	315933	2	8.786	855411	50.0