

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012624\
 Data File : VV033875.D
 Acq On : 26 Jan 2024 10:21
 Operator : SY/MD
 Sample : PB158608TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB608

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: VV033875.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	32	39	52	rBV	71424	79918	9.80%	1.181%
2	1.278	67	74	92	rBV	124561	160729	19.72%	2.376%
3	1.529	146	152	167	rVB	97699	119439	14.65%	1.765%
4	2.060	308	317	351	rVB	214626	330991	40.61%	4.892%
5	2.449	431	438	447	rBV3	2052	2918	0.36%	0.043%
6	2.555	467	471	481	rVB2	551	906	0.11%	0.013%
7	2.597	481	484	487	rBV	207	115	0.01%	0.002%
8	2.629	492	494	501	rVB2	106	81	0.01%	0.001%
9	2.696	509	515	517	rBV	173	169	0.02%	0.002%
10	2.735	524	527	529	rBV	140	93	0.01%	0.001%
11	2.902	576	579	582	rVB2	180	105	0.01%	0.002%
12	2.928	582	587	592	rBV2	140	193	0.02%	0.003%
13	2.960	592	597	602	rVB2	158	170	0.02%	0.003%
14	3.047	617	624	628	rBV	220	236	0.03%	0.003%
15	3.098	637	640	647	rBV2	189	155	0.02%	0.002%
16	3.217	673	677	680	rBV2	90	92	0.01%	0.001%
17	3.339	710	715	716	rBV2	106	101	0.01%	0.001%
18	3.429	740	743	745	rBV	144	89	0.01%	0.001%
19	3.445	745	748	752	rVB2	152	95	0.01%	0.001%
20	3.468	752	755	761	rVB2	126	124	0.02%	0.002%
21	3.661	809	815	817	rBV2	207	154	0.02%	0.002%
22	3.722	831	834	839	rVB2	121	125	0.02%	0.002%
23	3.751	839	843	845	rBV	110	96	0.01%	0.001%
24	3.783	845	853	880	rBV	52560	136802	16.78%	2.022%
25	4.249	982	998	1026	rBV	126580	321106	39.39%	4.746%
26	4.619	1112	1113	1116	rBV	181	80	0.01%	0.001%
27	4.706	1137	1140	1142	rBV	121	83	0.01%	0.001%
28	4.725	1142	1146	1150	rVB2	178	159	0.02%	0.002%
29	4.748	1150	1153	1155	rBV	151	80	0.01%	0.001%
30	4.783	1161	1164	1168	rBV	87	83	0.01%	0.001%
31	4.805	1168	1171	1175	rBV2	120	98	0.01%	0.001%
32	4.844	1180	1183	1185	rBV2	141	82	0.01%	0.001%
33	4.957	1201	1218	1260	rBV2	311016	815109	100.00%	12.048%
34	5.378	1347	1349	1353	rBV2	244	180	0.02%	0.003%
35	5.532	1384	1397	1428	rBV	257292	524935	64.40%	7.759%
36	5.831	1484	1490	1506	rVB3	1512	3227	0.40%	0.048%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak separation: 5

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 Title : VOC Analysis

37	5.989	1526	1539	1565	rBV	176400	363202	44.56%	5.368%
38	6.304	1628	1637	1640	rBV3	1354	2142	0.26%	0.032%
39	6.397	1657	1666	1699	rBV	52480	106332	13.05%	1.572%
40	6.735	1769	1771	1773	rBV	171	114	0.01%	0.002%
41	6.915	1816	1827	1855	rBV	103284	192296	23.59%	2.842%
42	7.120	1884	1891	1908	rBV	12833	21790	2.67%	0.322%
43	7.243	1918	1929	1956	rBV	377657	663214	81.37%	9.803%
44	7.555	2016	2026	2053	rBV	85564	157931	19.38%	2.334%
45	7.764	2088	2091	2094	rVB2	312	158	0.02%	0.002%
46	7.792	2096	2100	2103	rVB	286	196	0.02%	0.003%
47	7.863	2110	2122	2139	rBV	20283	36328	4.46%	0.537%
48	7.976	2147	2157	2162	rBV4	4027	5959	0.73%	0.088%
49	8.024	2163	2172	2198	rBV	194484	358231	43.95%	5.295%
50	8.249	2234	2242	2262	rBV	14278	26097	3.20%	0.386%
51	8.477	2310	2313	2316	rBV3	195	138	0.02%	0.002%
52	8.516	2322	2325	2328	rVB	233	141	0.02%	0.002%
53	8.535	2328	2331	2332	rBV	185	108	0.01%	0.002%
54	8.574	2339	2343	2345	rBV	132	105	0.01%	0.002%
55	8.619	2348	2357	2379	rBV	58943	94272	11.57%	1.393%
56	8.783	2398	2408	2446	rBV	383237	635604	77.98%	9.395%
57	9.043	2488	2489	2492	rVB	197	100	0.01%	0.001%
58	9.069	2492	2497	2501	rBV3	379	519	0.06%	0.008%
59	9.124	2508	2514	2518	rBV	211	243	0.03%	0.004%
60	9.304	2567	2570	2573	rVB	155	102	0.01%	0.002%
61	9.352	2580	2585	2590	rBV2	398	494	0.06%	0.007%
62	9.497	2623	2630	2644	rVB4	2871	5179	0.64%	0.077%
63	9.599	2660	2662	2665	rVB2	246	137	0.02%	0.002%
64	9.853	2738	2741	2745	rBV2	158	98	0.01%	0.001%
65	9.927	2761	2764	2767	rBV	126	102	0.01%	0.002%
66	9.985	2778	2782	2783	rBV	143	89	0.01%	0.001%
67	10.014	2789	2791	2800	rVB	187	156	0.02%	0.002%
68	10.098	2814	2817	2822	rBV2	168	169	0.02%	0.002%
69	10.152	2822	2834	2850	rBV	229598	357833	43.90%	5.289%
70	10.300	2877	2880	2883	rVB2	208	121	0.01%	0.002%
71	10.320	2883	2886	2892	rVB2	102	102	0.01%	0.002%
72	10.352	2892	2896	2901	rBV2	181	196	0.02%	0.003%
73	10.378	2901	2904	2906	rBV	198	124	0.02%	0.002%
74	10.497	2937	2941	2945	rVB2	187	139	0.02%	0.002%
75	10.516	2945	2947	2950	rBV	143	102	0.01%	0.002%
76	10.590	2967	2970	2972	rBV	134	87	0.01%	0.001%

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Stop Thrs : 0

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Peak separation: 5

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 Title : VOC Analysis

77	10.625	2978	2981	2987	rBV2	239	287	0.04%	0.004%
78	10.776	3025	3028	3032	rBV2	99	87	0.01%	0.001%
79	10.834	3043	3046	3051	rBV	147	133	0.02%	0.002%
80	11.185	3144	3155	3181	rBV	406571	630971	77.41%	9.326%
81	11.503	3250	3254	3256	rBV	224	184	0.02%	0.003%
82	11.561	3260	3272	3297	rVV	384380	598348	73.41%	8.844%
83	11.847	3359	3361	3363	rBV	157	83	0.01%	0.001%
84	11.924	3381	3385	3388	rBV2	219	165	0.02%	0.002%
85	12.056	3423	3426	3429	rBV2	192	131	0.02%	0.002%
86	12.101	3437	3440	3443	rBV	230	130	0.02%	0.002%
87	12.123	3444	3447	3452	rVB	240	195	0.02%	0.003%
88	12.149	3452	3455	3457	rBV2	212	132	0.02%	0.002%
89	12.197	3466	3470	3474	rBV2	204	185	0.02%	0.003%
90	12.252	3480	3487	3489	rBV2	203	248	0.03%	0.004%
91	12.400	3530	3533	3537	rBV	220	158	0.02%	0.002%
92	12.930	3695	3698	3699	rBV	153	95	0.01%	0.001%
93	13.043	3726	3733	3735	rBV2	234	302	0.04%	0.004%
94	13.210	3781	3785	3790	rBV4	417	458	0.06%	0.007%
95	13.451	3856	3860	3873	rVB3	1788	2580	0.32%	0.038%
96	13.545	3885	3889	3893	rBV2	323	351	0.04%	0.005%
97	13.747	3950	3952	3954	rBV2	301	110	0.01%	0.002%
98	13.850	3981	3984	3988	rBV2	196	180	0.02%	0.003%
99	14.175	4081	4085	4090	rBV3	258	242	0.03%	0.004%
100	14.249	4103	4108	4112	rBV3	343	369	0.05%	0.005%

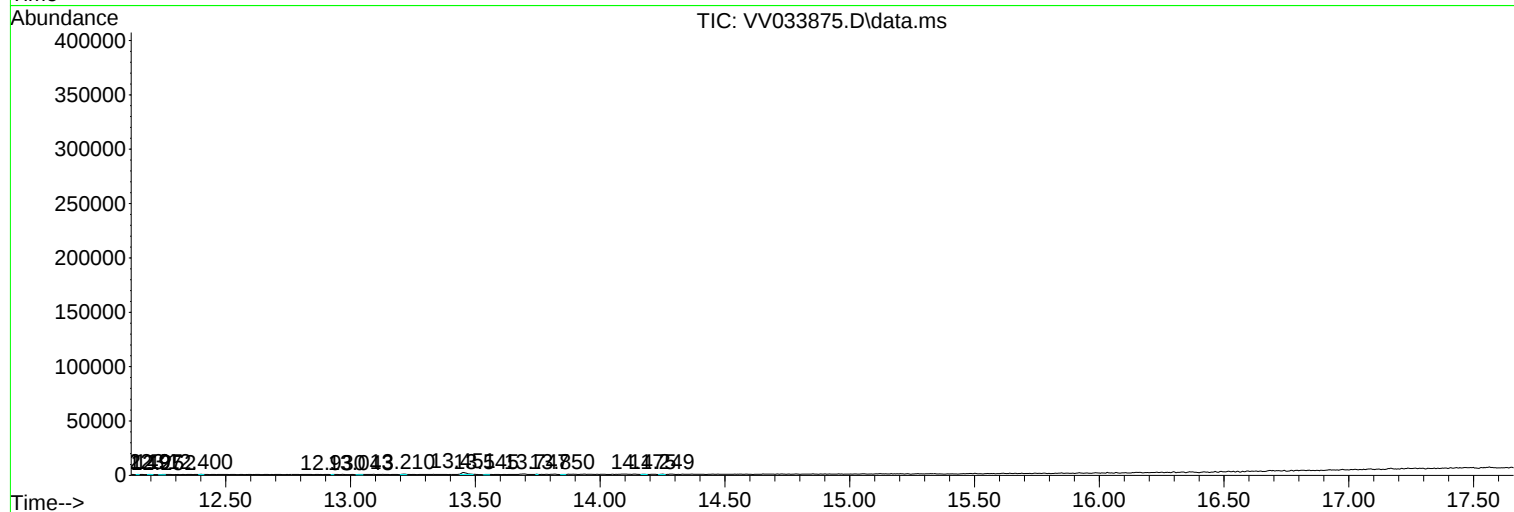
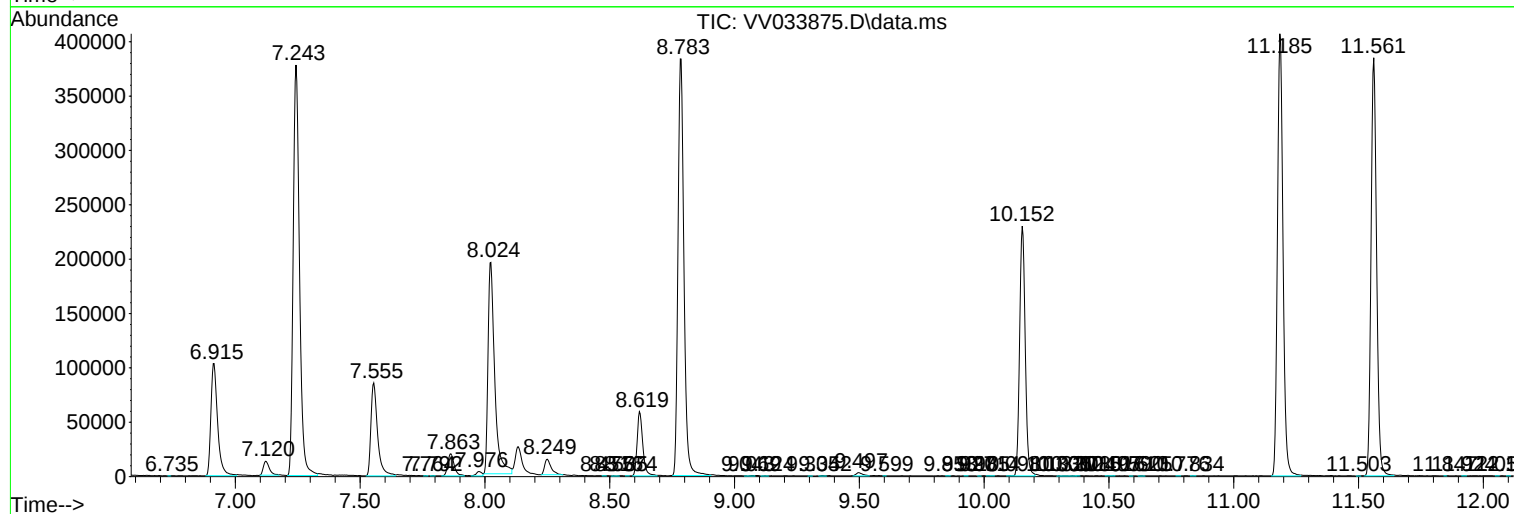
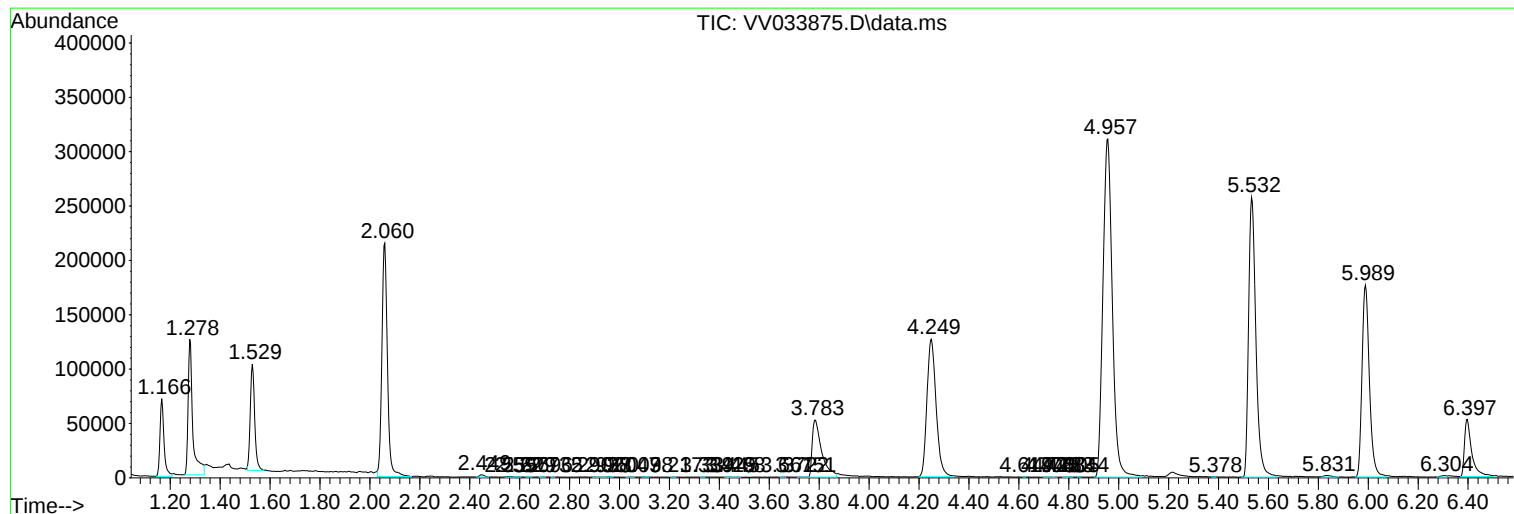
Sum of corrected areas: 6765692

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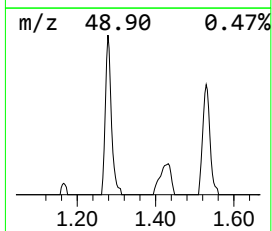
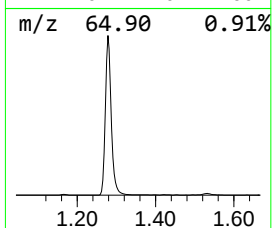
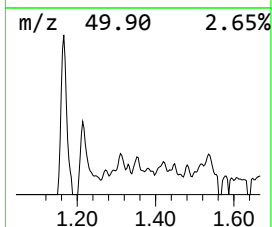
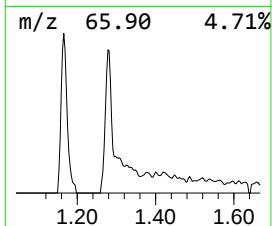
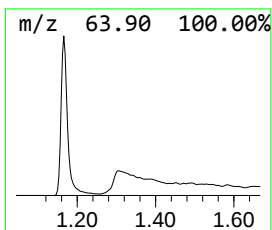
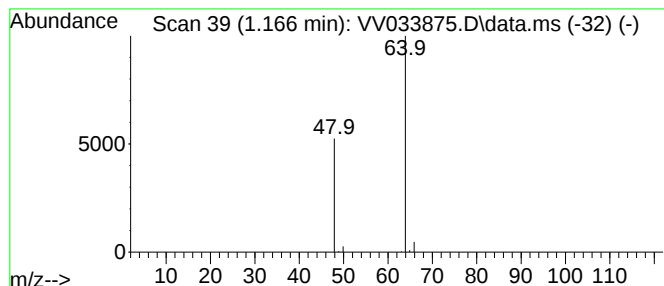
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.166	7.61 ug/L	79918	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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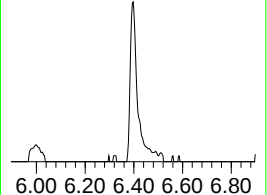
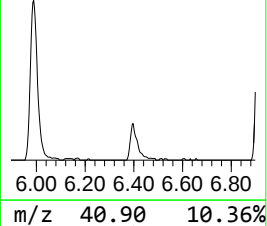
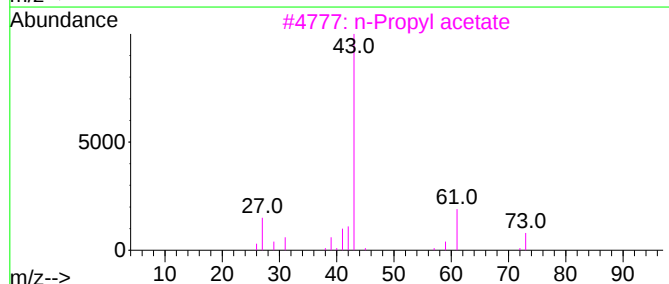
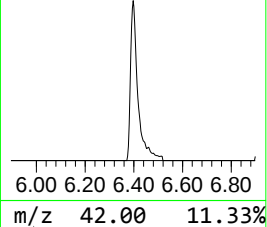
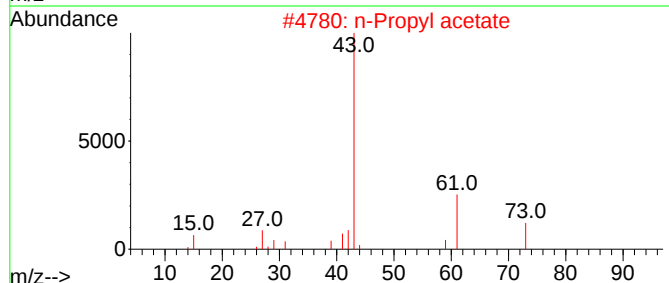
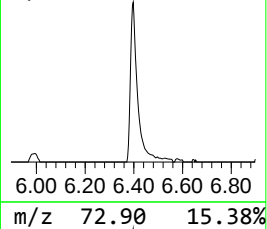
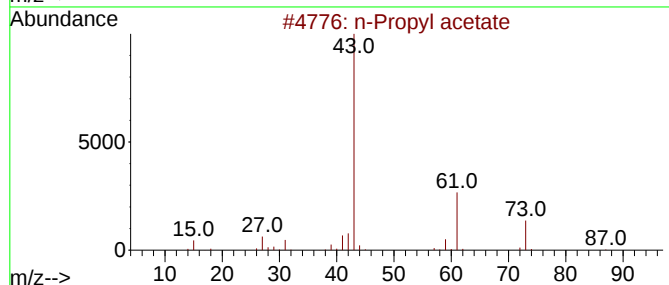
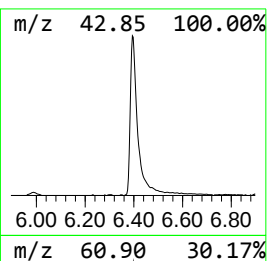
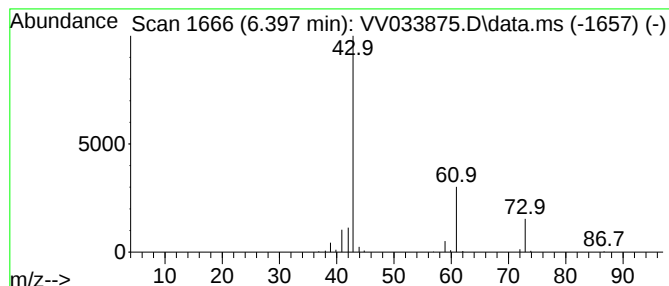
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.397	10.13 ug/L	106332	1,4-Difluorobenzene	5.532

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	72
3	n-Propyl acetate			102	C5H10O2	000109-60-4	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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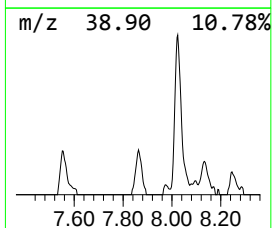
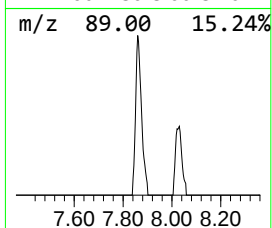
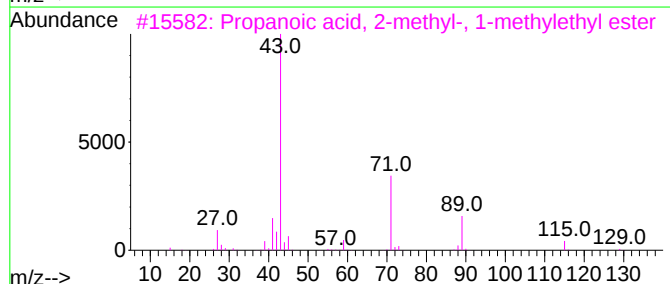
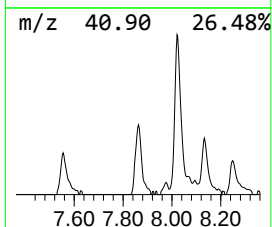
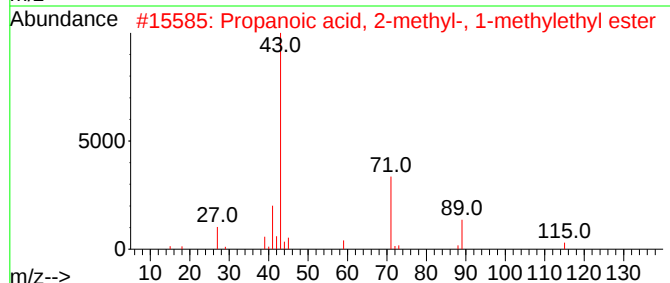
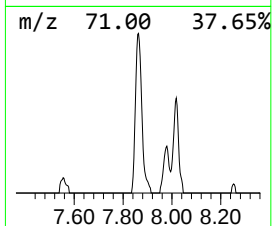
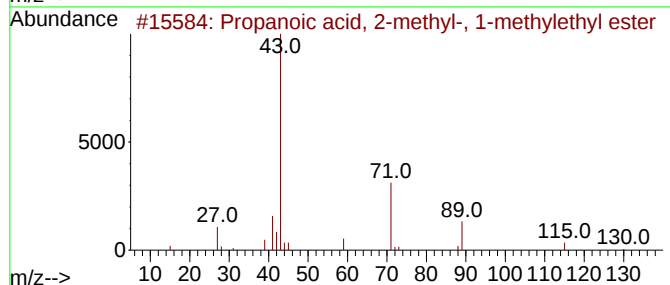
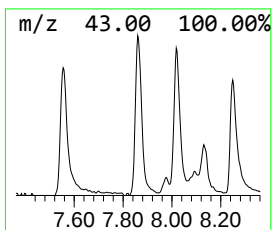
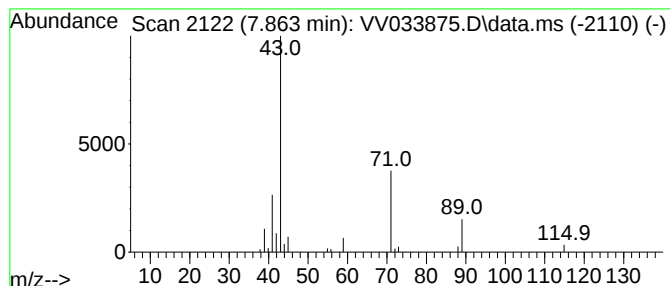
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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	2.86 ug/L	36328	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



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ClientSampleId :
VLEB608

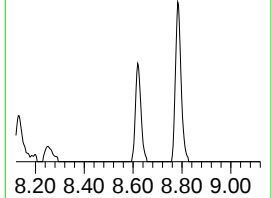
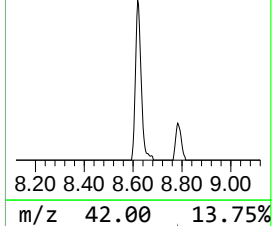
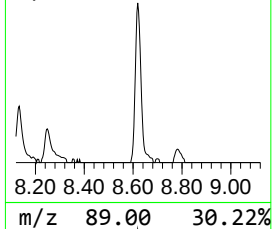
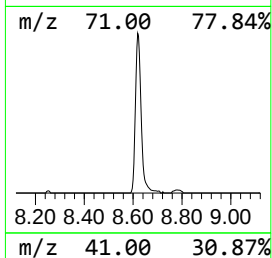
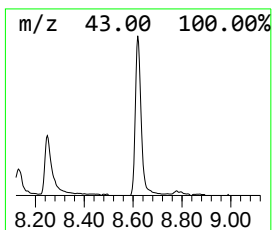
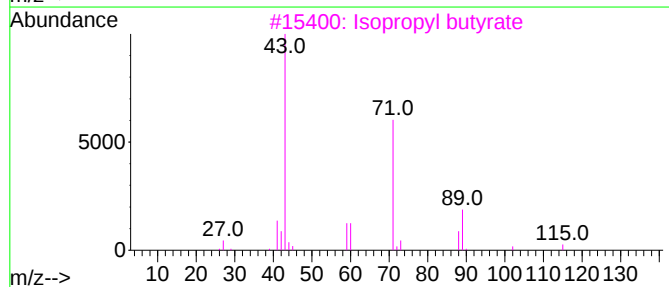
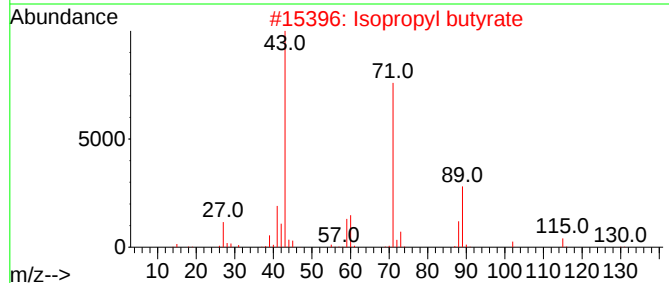
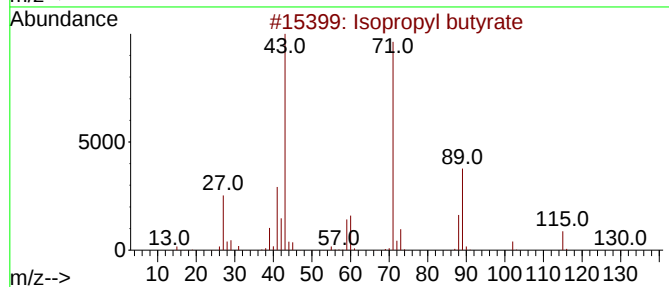
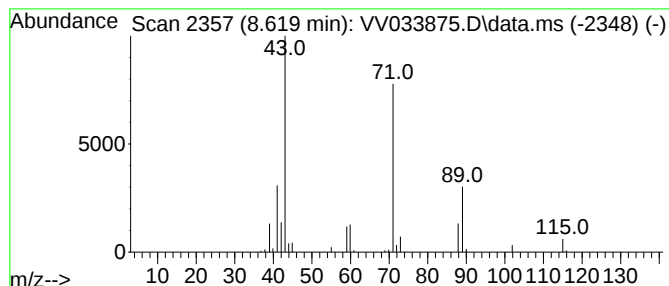
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Quant Title : VOC Analysis

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

Peak Number 5 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	7.42 ug/L	94272	Chlorobenzene-d5	8.786

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	78
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012624\
Data File : VV033875.D
Acq On : 26 Jan 2024 10:21
Operator : SY/MD
Sample : PB158608TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB608

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.166	7.6	ug/L	79918	1	5.532	524935	50.0
n-Propyl acetate	6.397	10.1	ug/L	106332	1	5.532	524935	50.0
Propanoic acid,...	7.863	2.9	ug/L	36328	2	8.786	635604	50.0
Isopropyl butyrate	8.619	7.4	ug/L	94272	2	8.786	635604	50.0