

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032724\
 Data File : VV034871.D
 Acq On : 27 Mar 2024 17:41
 Operator : SY/MD
 Sample : PB159798TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 20 Sample Multiplier: 1

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\SFAMVLM032624WMA.M

Title : VOC Analysis

Signal : TIC: VV034871.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	67	74	87	rBV	157575	164323	12.83%	1.544%
2	1.529	145	152	166	rVB	150256	177980	13.89%	1.672%
3	2.060	307	317	329	rBV	273765	404615	31.58%	3.802%
4	2.513	456	458	462	rVB3	499	242	0.02%	0.002%
5	2.529	462	463	464	rBV3	322	118	0.01%	0.001%
6	2.629	492	494	495	rBV	332	170	0.01%	0.002%
7	2.680	508	510	512	rBV	419	242	0.02%	0.002%
8	2.716	519	521	524	rBV	197	120	0.01%	0.001%
9	2.757	530	534	536	rBV	405	265	0.02%	0.002%
10	2.883	571	573	574	rBV	276	114	0.01%	0.001%
11	3.114	636	645	647	rBV5	2753	3772	0.29%	0.035%
12	3.365	720	723	725	rBB2	326	180	0.01%	0.002%
13	3.375	725	726	728	rVB	466	114	0.01%	0.001%
14	3.397	731	733	735	rBV2	321	150	0.01%	0.001%
15	3.410	735	737	740	rBV2	411	291	0.02%	0.003%
16	3.442	745	747	750	rBV3	173	139	0.01%	0.001%
17	3.487	758	761	766	rBV4	540	389	0.03%	0.004%
18	3.526	769	773	776	rBV2	274	150	0.01%	0.001%
19	3.577	786	789	791	rBV3	369	219	0.02%	0.002%
20	3.600	794	796	798	rBV	423	137	0.01%	0.001%
21	3.661	813	815	818	rVB	256	117	0.01%	0.001%
22	3.683	818	822	824	rBV2	274	195	0.02%	0.002%
23	3.712	828	831	835	rVB2	294	173	0.01%	0.002%
24	3.728	835	836	841	rVB	215	131	0.01%	0.001%
25	3.780	844	852	891	rBV	107972	301356	23.52%	2.831%
26	4.246	982	997	1031	rBV	211343	545414	42.57%	5.125%
27	4.561	1093	1095	1098	rBV2	272	148	0.01%	0.001%
28	4.603	1105	1108	1111	rBV2	569	510	0.04%	0.005%
29	4.648	1120	1122	1126	rVB3	312	197	0.02%	0.002%
30	4.725	1144	1146	1149	rBV3	267	135	0.01%	0.001%
31	4.886	1192	1196	1197	rBV2	222	153	0.01%	0.001%
32	4.953	1201	1217	1247	rBV2	475139	1281267	100.00%	12.039%
33	5.532	1386	1397	1424	rBV	392579	819577	63.97%	7.701%
34	5.831	1481	1490	1510	rVB3	9130	21735	1.70%	0.204%
35	5.941	1521	1524	1525	rBV2	414	199	0.02%	0.002%
36	5.986	1526	1538	1565	rBV	295145	615046	48.00%	5.779%

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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\SFAMVLM032624WMA.M
 Title : VOC Analysis

37	6.394	1657	1665	1694	rBV	80602	167394	13.06%	1.573%
38	6.806	1791	1793	1794	rBV	405	149	0.01%	0.001%
39	6.863	1808	1811	1814	rBV2	305	223	0.02%	0.002%
40	6.912	1816	1826	1857	rBV	152550	293881	22.94%	2.761%
41	7.121	1884	1891	1906	rBV2	19640	33840	2.64%	0.318%
42	7.243	1918	1929	1967	rBV	540349	943228	73.62%	8.862%
43	7.555	2016	2026	2051	rBV	125809	240260	18.75%	2.257%
44	7.863	2112	2122	2140	rBV2	27284	47243	3.69%	0.444%
45	8.021	2163	2171	2198	rBV	354658	654035	51.05%	6.145%
46	8.249	2237	2242	2260	rVB	20440	36951	2.88%	0.347%
47	8.619	2348	2357	2379	rBV	77607	128947	10.06%	1.212%
48	8.783	2398	2408	2446	rBV	646264	1055681	82.39%	9.919%
49	9.188	2532	2534	2536	rBV2	424	238	0.02%	0.002%
50	9.243	2549	2551	2552	rBV	416	175	0.01%	0.002%
51	9.783	2717	2719	2721	rBV	222	116	0.01%	0.001%
52	9.799	2721	2724	2727	rBV2	355	256	0.02%	0.002%
53	9.838	2734	2736	2741	rBV4	407	285	0.02%	0.003%
54	9.989	2779	2783	2785	rBV3	483	357	0.03%	0.003%
55	10.027	2791	2795	2796	rBV	337	195	0.02%	0.002%
56	10.056	2802	2804	2807	rBV3	377	182	0.01%	0.002%
57	10.153	2822	2834	2858	rBV	458203	738834	57.66%	6.942%
58	10.490	2934	2939	2943	rBV3	435	474	0.04%	0.004%
59	10.526	2947	2950	2954	rBV2	331	272	0.02%	0.003%
60	10.545	2954	2956	2957	rBV	407	148	0.01%	0.001%
61	10.667	2990	2994	2996	rBV2	203	155	0.01%	0.001%
62	10.680	2996	2998	3001	rVB	322	162	0.01%	0.002%
63	10.776	3026	3028	3030	rBV2	252	143	0.01%	0.001%
64	10.854	3048	3052	3054	rBV3	377	263	0.02%	0.002%
65	10.956	3082	3084	3085	rBV3	261	129	0.01%	0.001%
66	11.024	3103	3105	3106	rBV2	283	134	0.01%	0.001%
67	11.069	3116	3119	3122	rBV	300	290	0.02%	0.003%
68	11.098	3125	3128	3130	rBV	259	139	0.01%	0.001%
69	11.185	3144	3155	3177	rBV	638861	995580	77.70%	9.354%
70	11.455	3237	3239	3244	rBV4	436	390	0.03%	0.004%
71	11.487	3244	3249	3254	rVB3	614	557	0.04%	0.005%
72	11.513	3254	3257	3260	rBV4	541	374	0.03%	0.004%
73	11.558	3260	3271	3289	rBV	593920	953960	74.45%	8.963%
74	11.802	3341	3347	3352	rVB5	961	1004	0.08%	0.009%
75	11.828	3352	3355	3357	rBV	454	312	0.02%	0.003%
76	11.931	3385	3387	3389	rBV2	406	225	0.02%	0.002%

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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\SFAMVLM032624WMA.M
 Title : VOC Analysis

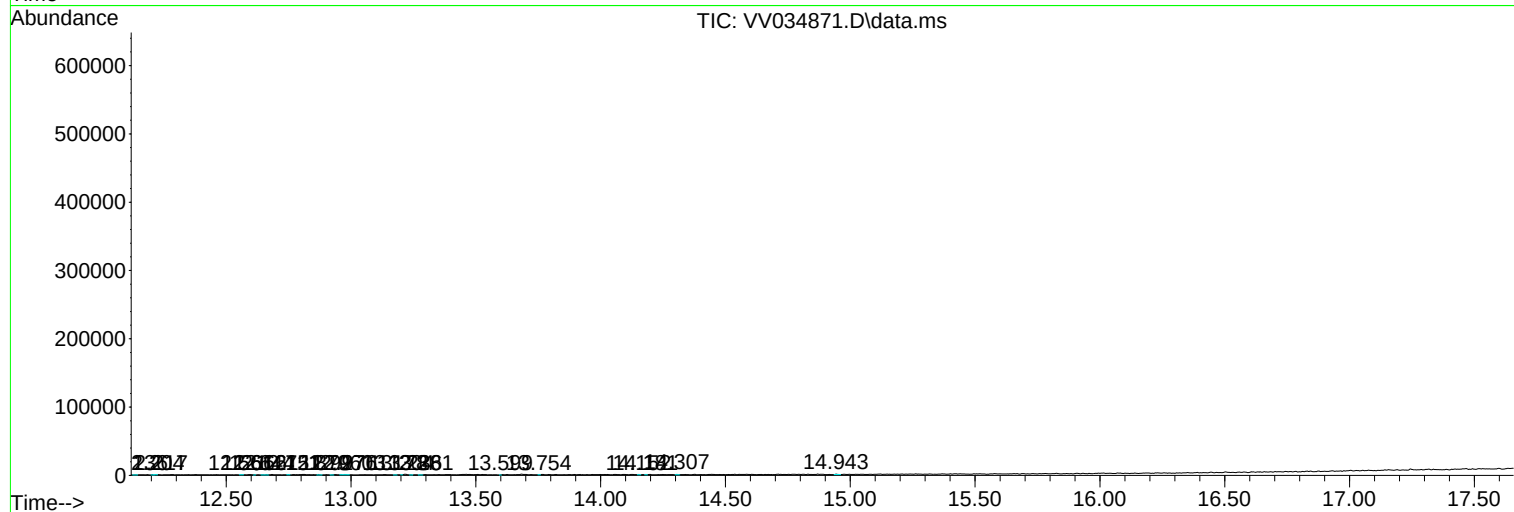
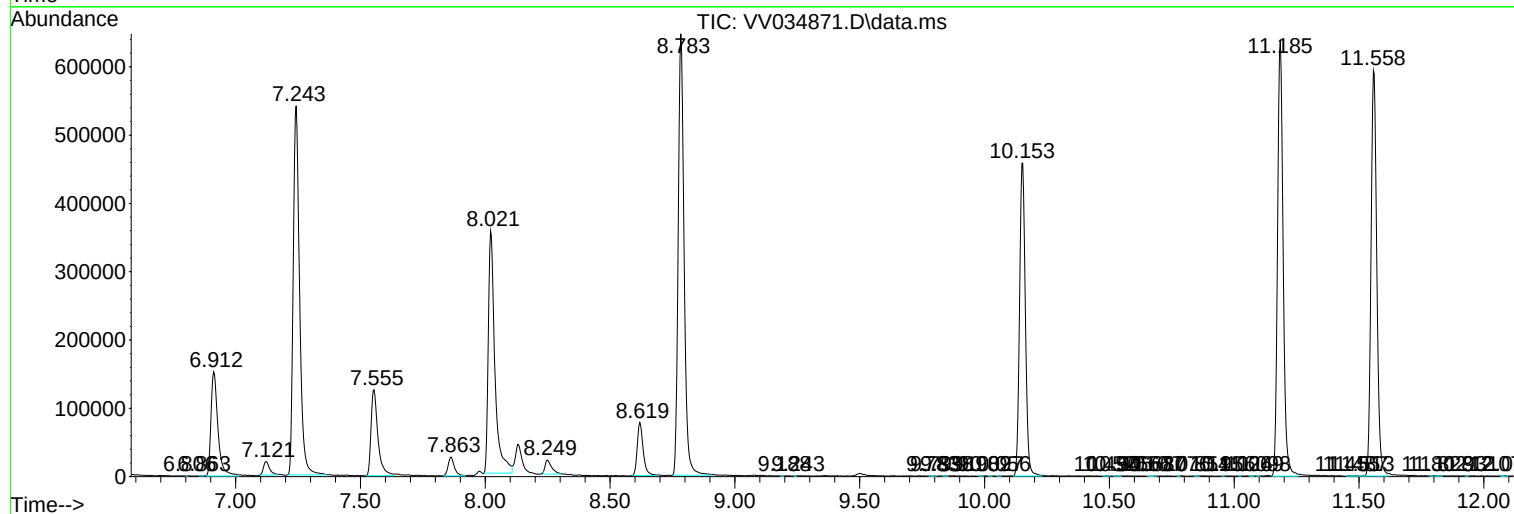
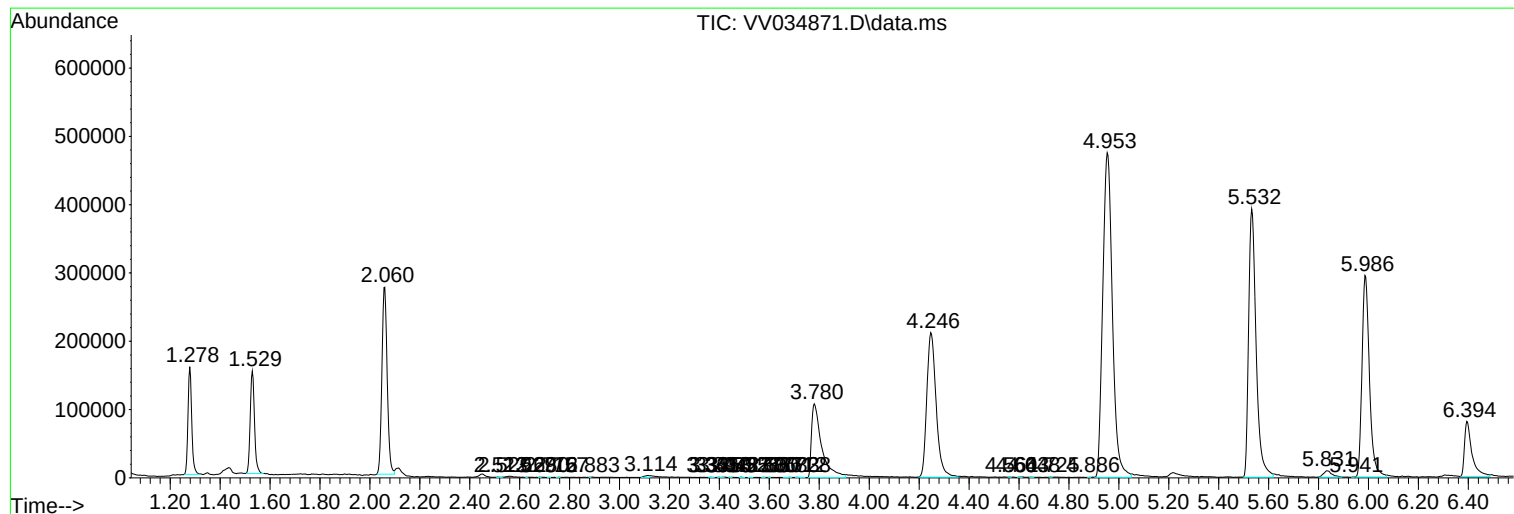
77	12.072	3429	3431	3432	rBV2	323	146	0.01%	0.001%
78	12.082	3432	3434	3439	rVB3	675	480	0.04%	0.005%
79	12.136	3447	3451	3454	rBV2	297	165	0.01%	0.002%
80	12.204	3470	3472	3474	rBV2	339	190	0.01%	0.002%
81	12.217	3474	3476	3479	rVV2	284	132	0.01%	0.001%
82	12.561	3580	3583	3586	rBV2	448	261	0.02%	0.002%
83	12.612	3598	3599	3601	rVB	473	125	0.01%	0.001%
84	12.644	3607	3609	3612	rBV2	417	296	0.02%	0.003%
85	12.661	3612	3614	3617	rBV	417	269	0.02%	0.003%
86	12.751	3639	3642	3644	rVB	290	119	0.01%	0.001%
87	12.870	3677	3679	3684	rVB2	623	367	0.03%	0.003%
88	12.927	3693	3697	3698	rBV2	428	221	0.02%	0.002%
89	12.960	3705	3707	3710	rVB3	450	177	0.01%	0.002%
90	12.976	3710	3712	3718	rBV3	512	417	0.03%	0.004%
91	13.178	3772	3775	3777	rBV	297	223	0.02%	0.002%
92	13.204	3781	3783	3784	rBV	362	170	0.01%	0.002%
93	13.236	3792	3793	3797	rVB	348	187	0.01%	0.002%
94	13.281	3803	3807	3809	rBV2	334	277	0.02%	0.003%
95	13.599	3904	3906	3907	rBV2	383	150	0.01%	0.001%
96	13.754	3952	3954	3956	rBV	278	200	0.02%	0.002%
97	14.152	4076	4078	4081	rBV2	393	141	0.01%	0.001%
98	14.181	4085	4087	4089	rBV2	368	160	0.01%	0.002%
99	14.307	4123	4126	4129	rBV3	511	365	0.03%	0.003%
100	14.943	4321	4324	4330	rBV3	754	563	0.04%	0.005%

Sum of corrected areas: 10643065

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ALS Vial : 20 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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



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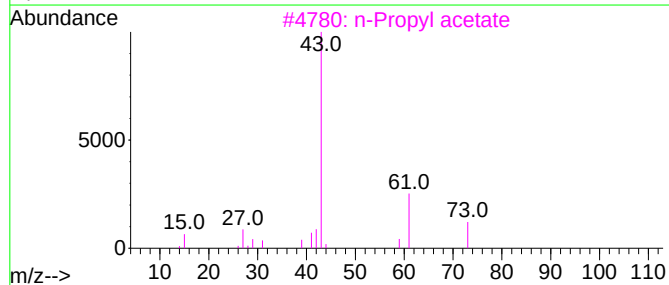
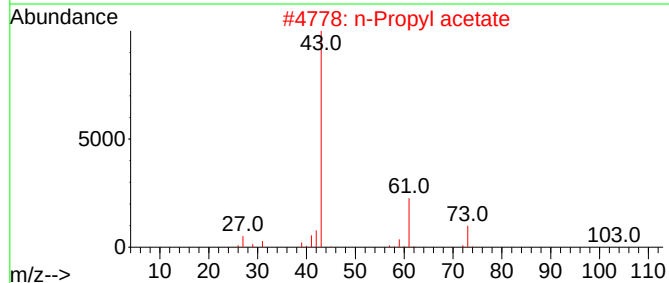
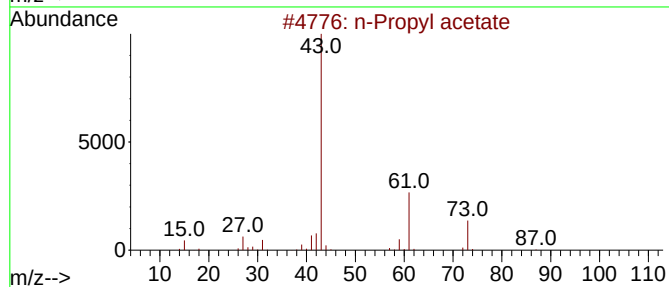
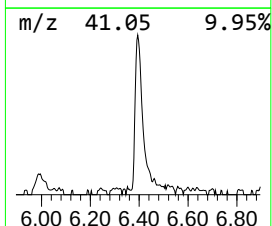
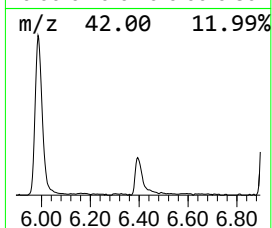
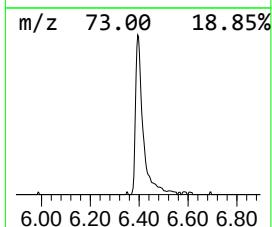
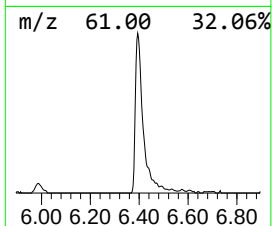
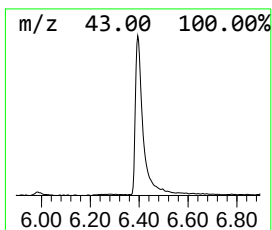
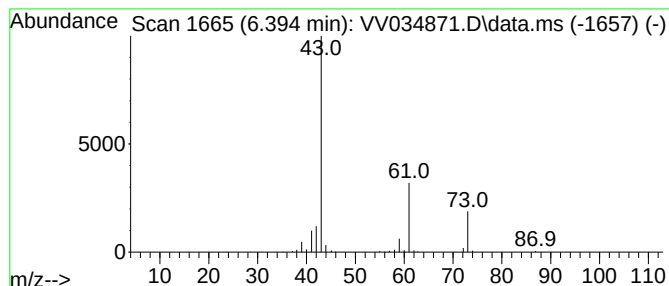
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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	10.21 ug/L	167394	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	64
3	n-Propyl acetate			102	C5H10O2	000109-60-4	50
4	n-Propyl acetate			102	C5H10O2	000109-60-4	38
5	Isopropyl acetate			102	C5H10O2	000108-21-4	36



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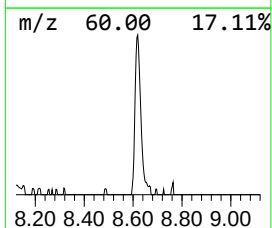
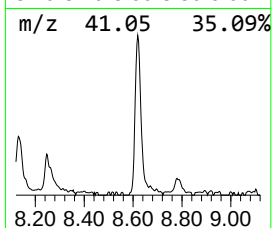
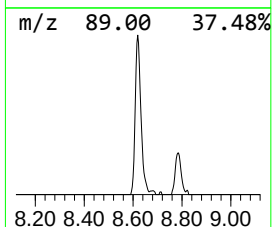
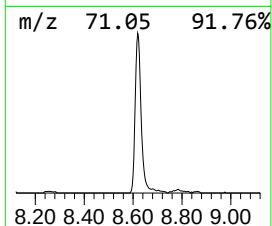
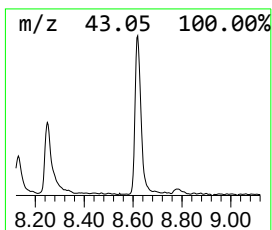
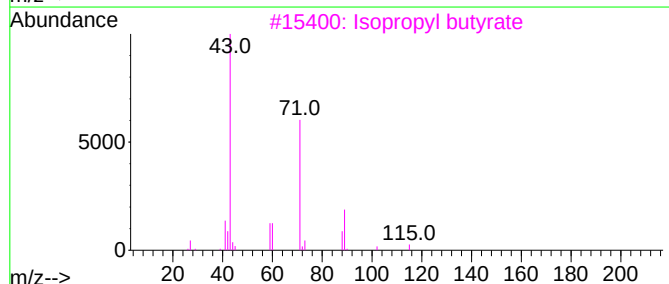
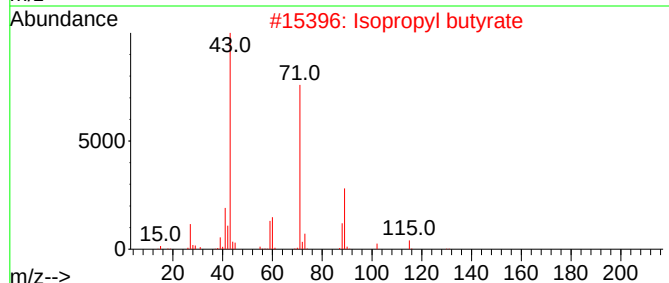
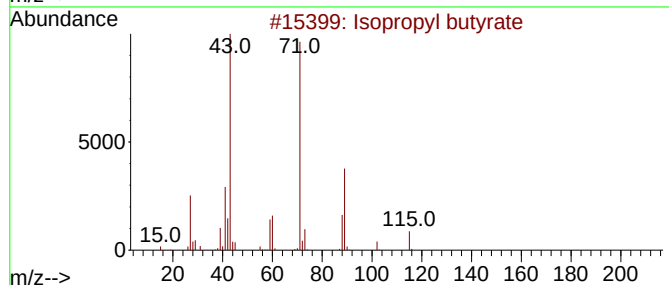
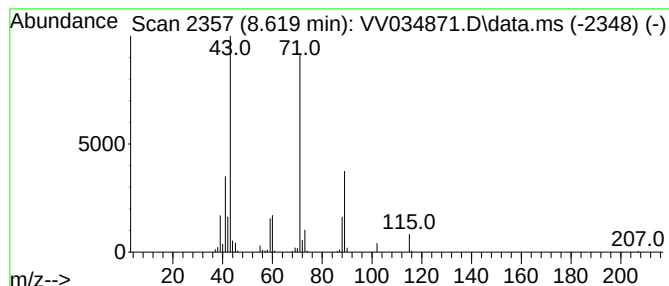
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	6.11 ug/L	128947	Chlorobenzene-d5	8.783

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			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64



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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	6.394	10.2	ug/L	167394	1	5.532	819577	50.0
Isopropyl butyrate	8.619	6.1	ug/L	128947	2	8.783	1055680	50.0