

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW121922\
 Data File : VW029712.D
 Acq On : 19 Dec 2022 11:32
 Operator : SY/MD
 Sample : N6075-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGSL8

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: VW029712.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	96	rVB	218802	219485	14.77%	1.763%
2	1.561	155	162	175	rVB	181553	206691	13.91%	1.660%
3	2.105	319	331	344	rBV	358968	516312	34.74%	4.146%
4	2.282	381	386	389	rBV4	956	1025	0.07%	0.008%
5	2.503	445	455	467	rBV2	8385	13905	0.94%	0.112%
6	2.606	477	487	501	rBV4	742	1956	0.13%	0.016%
7	2.934	583	589	594	rBV	181	187	0.01%	0.002%
8	3.333	707	713	717	rVV3	307	275	0.02%	0.002%
9	3.468	752	755	762	rVB2	156	200	0.01%	0.002%
10	3.513	764	769	774	rBV2	190	184	0.01%	0.001%
11	3.728	831	836	838	rVV2	258	185	0.01%	0.001%
12	3.780	847	852	856	rVV	205	194	0.01%	0.002%
13	3.876	872	882	916	rBV	103194	312631	21.03%	2.511%
14	4.185	975	978	981	rVB3	567	385	0.03%	0.003%
15	4.339	1008	1026	1069	rBV	228570	576931	38.81%	4.633%
16	4.696	1133	1137	1143	rVB2	307	347	0.02%	0.003%
17	4.780	1161	1163	1166	rVB2	335	181	0.01%	0.001%
18	4.963	1216	1220	1226	rVB	259	303	0.02%	0.002%
19	5.040	1226	1244	1281	rBV2	565065	1486429	100.00%	11.937%
20	5.285	1311	1320	1340	rVB3	6028	13802	0.93%	0.111%
21	5.468	1374	1377	1380	rBV2	627	451	0.03%	0.004%
22	5.484	1380	1382	1390	rVB4	458	539	0.04%	0.004%
23	5.548	1398	1402	1403	rBV2	284	209	0.01%	0.002%
24	5.609	1408	1421	1456	rBV	533189	1093632	73.57%	8.783%
25	5.899	1501	1511	1529	rVB5	5679	13114	0.88%	0.105%
26	6.063	1546	1562	1598	rBV	322534	666988	44.87%	5.356%
27	6.188	1598	1601	1602	rBV3	366	207	0.01%	0.002%
28	6.246	1618	1619	1622	rVB3	682	298	0.02%	0.002%
29	6.310	1636	1639	1642	rVB2	527	290	0.02%	0.002%
30	6.355	1642	1653	1657	rBV	3303	5601	0.38%	0.045%
31	6.465	1678	1687	1711	rBV	44647	93611	6.30%	0.752%
32	6.619	1733	1735	1739	rVB4	707	388	0.03%	0.003%
33	6.838	1801	1803	1807	rVB3	367	206	0.01%	0.002%
34	6.937	1828	1834	1835	rBV2	340	204	0.01%	0.002%
35	6.979	1835	1847	1876	rBV	163063	302653	20.36%	2.431%
36	7.101	1883	1885	1888	rVB2	555	328	0.02%	0.003%

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

37	7.182	1897	1910	1922	rBV	19452	35161	2.37%	0.282%
38	7.307	1937	1949	1971	rBV	704555	1232065	82.89%	9.894%
39	7.568	2028	2030	2033	rVB	434	186	0.01%	0.001%
40	7.613	2033	2044	2072	rBV	124647	225646	15.18%	1.812%
41	7.767	2088	2092	2095	rBV3	335	274	0.02%	0.002%
42	7.921	2130	2140	2153	rBV	24601	43245	2.91%	0.347%
43	8.031	2160	2174	2179	rBV6	3076	5439	0.37%	0.044%
44	8.085	2180	2191	2216	rVV	371728	680124	45.76%	5.462%
45	8.191	2217	2224	2238	rVB	20121	35433	2.38%	0.285%
46	8.307	2252	2260	2273	rVB2	6053	11395	0.77%	0.092%
47	8.413	2286	2293	2299	rBV6	1408	1969	0.13%	0.016%
48	8.503	2317	2321	2324	rBV4	485	394	0.03%	0.003%
49	8.519	2324	2326	2329	rVB3	351	203	0.01%	0.002%
50	8.564	2337	2340	2347	rVB3	428	392	0.03%	0.003%
51	8.603	2347	2352	2354	rBV	425	283	0.02%	0.002%
52	8.677	2365	2375	2393	rVV2	44789	72736	4.89%	0.584%
53	8.773	2403	2405	2412	rVB3	328	249	0.02%	0.002%
54	8.844	2412	2427	2466	rBV	788008	1308684	88.04%	10.510%
55	8.989	2471	2472	2473	rBV	561	210	0.01%	0.002%
56	9.047	2487	2490	2493	rVB2	469	254	0.02%	0.002%
57	9.133	2506	2517	2523	rBV5	2559	4529	0.30%	0.036%
58	9.384	2591	2595	2597	rBV3	346	265	0.02%	0.002%
59	9.539	2635	2643	2656	rBV9	2543	4982	0.34%	0.040%
60	9.702	2689	2694	2700	rVB4	378	419	0.03%	0.003%
61	9.928	2759	2764	2768	rBV4	457	523	0.04%	0.004%
62	10.162	2827	2837	2841	rBV2	18196	26827	1.80%	0.215%
63	10.207	2841	2851	2875	rVV	460218	725896	48.83%	5.829%
64	10.297	2876	2879	2883	rVB3	466	340	0.02%	0.003%
65	10.371	2893	2902	2909	rVV4	1579	2323	0.16%	0.019%
66	10.436	2920	2922	2926	rBV	224	180	0.01%	0.001%
67	10.526	2947	2950	2955	rVV3	500	463	0.03%	0.004%
68	10.567	2955	2963	2980	rVB	9407	14836	1.00%	0.119%
69	10.648	2985	2988	2994	rVB2	273	211	0.01%	0.002%
70	10.735	3011	3015	3019	rBV3	327	249	0.02%	0.002%
71	10.850	3044	3051	3057	rVB3	549	520	0.03%	0.004%
72	10.905	3063	3068	3070	rBV	628	540	0.04%	0.004%
73	10.937	3076	3078	3084	rVB2	258	226	0.02%	0.002%
74	11.175	3143	3152	3159	rBV4	935	1435	0.10%	0.012%
75	11.236	3159	3171	3196	rBV	879424	1357480	91.32%	10.901%
76	11.500	3249	3253	3258	rBV	258	205	0.01%	0.002%

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77	11.561	3269	3272	3275	rBV2	398	229	0.02%	0.002%
78	11.612	3275	3288	3312	rBV	707158	1110261	74.69%	8.916%
79	11.815	3348	3351	3352	rBV2	312	200	0.01%	0.002%
80	11.908	3377	3380	3384	rBV	328	300	0.02%	0.002%
81	11.998	3406	3408	3414	rVB2	356	282	0.02%	0.002%
82	12.175	3461	3463	3467	rVB2	398	191	0.01%	0.002%
83	12.243	3476	3484	3492	rBV2	1469	2031	0.14%	0.016%
84	12.336	3507	3513	3515	rBV3	459	495	0.03%	0.004%
85	12.400	3529	3533	3535	rBV3	303	266	0.02%	0.002%
86	12.535	3572	3575	3580	rVB2	390	301	0.02%	0.002%
87	12.564	3580	3584	3585	rBV2	283	203	0.01%	0.002%
88	12.644	3600	3609	3614	rBV4	1102	1323	0.09%	0.011%
89	12.738	3635	3638	3640	rBV2	266	211	0.01%	0.002%
90	12.805	3657	3659	3666	rVB2	395	275	0.02%	0.002%
91	12.847	3669	3672	3675	rBV3	370	213	0.01%	0.002%
92	13.072	3739	3742	3748	rVB3	353	348	0.02%	0.003%
93	13.149	3762	3766	3770	rVB3	375	300	0.02%	0.002%
94	13.178	3774	3775	3779	rBV2	267	185	0.01%	0.001%
95	13.249	3795	3797	3804	rVB5	1413	1403	0.09%	0.011%
96	13.316	3815	3818	3820	rBV	544	338	0.02%	0.003%
97	13.329	3820	3822	3824	rVV	303	188	0.01%	0.002%
98	13.426	3849	3852	3855	rBV4	342	265	0.02%	0.002%
99	13.497	3865	3874	3881	rBV	3527	5109	0.34%	0.041%
100	14.355	4139	4141	4143	rBV2	495	247	0.02%	0.002%

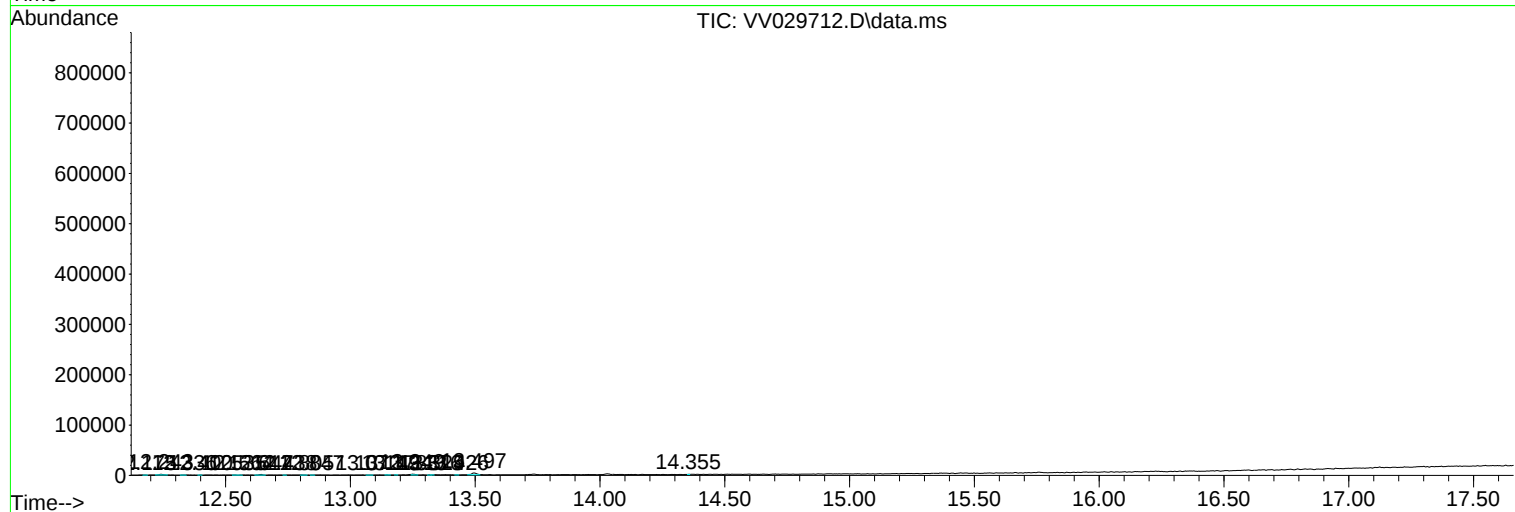
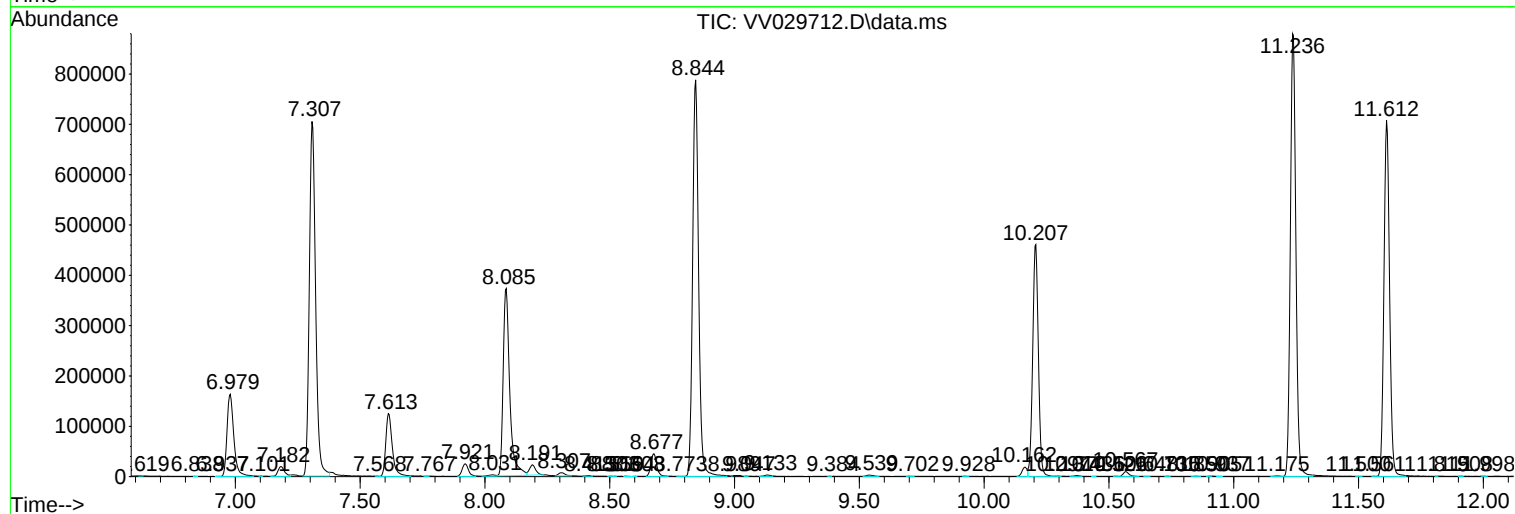
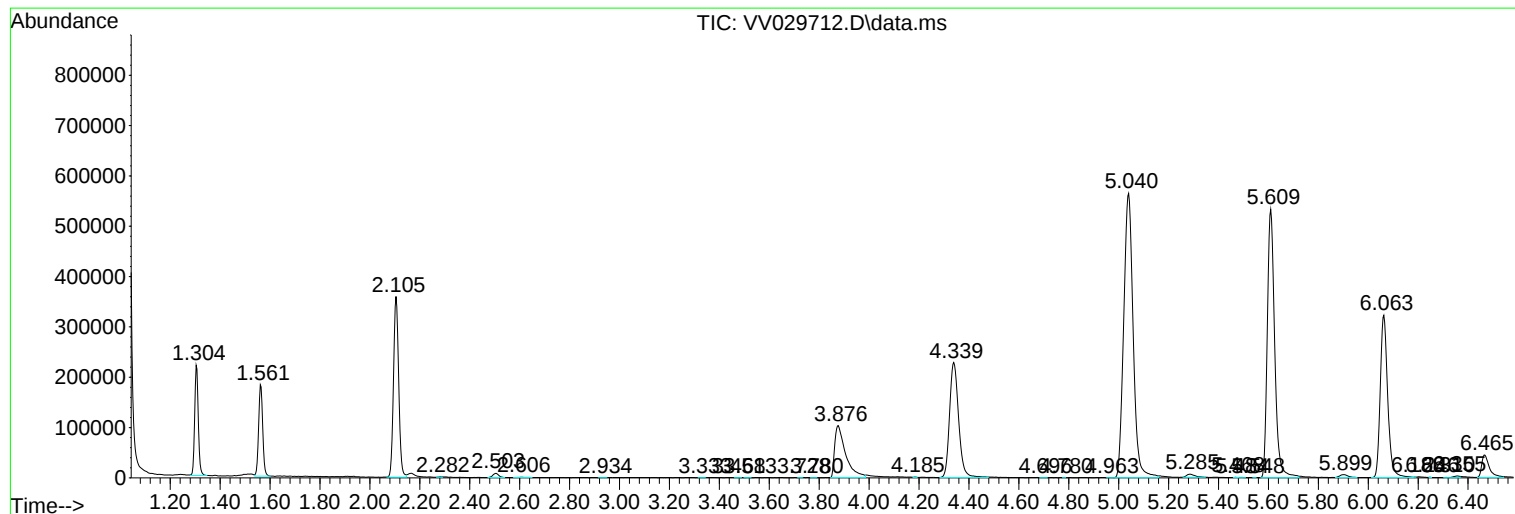
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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



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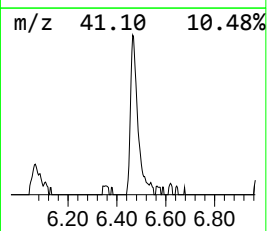
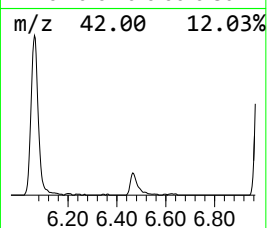
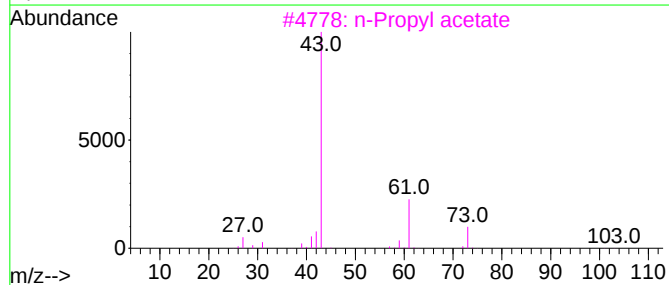
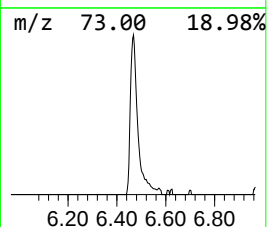
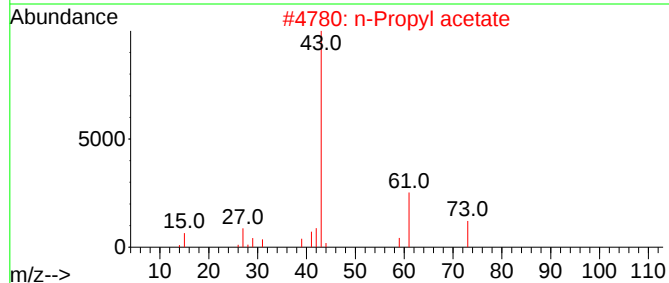
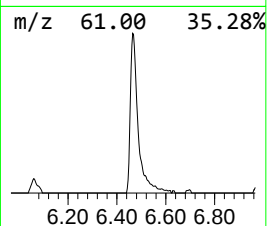
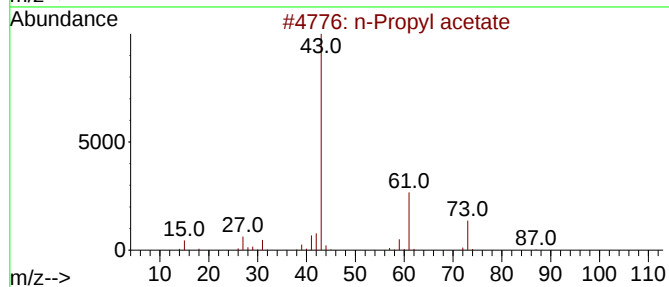
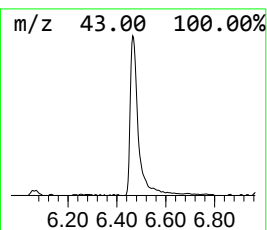
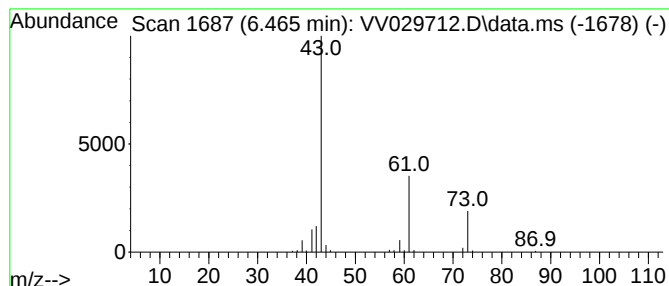
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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.
6.465	4.28 ug/L	93611	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	64
3	n-Propyl acetate			102	C5H10O2	000109-60-4	50
4	n-Propyl acetate			102	C5H10O2	000109-60-4	38
5	Propanal, 2,3-dihydroxy-, (S)-			90	C3H6O3	000497-09-6	36



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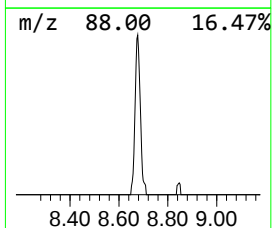
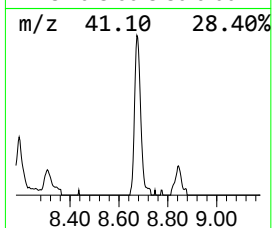
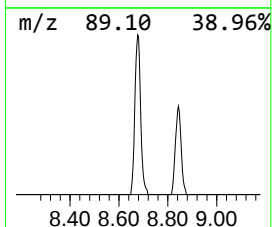
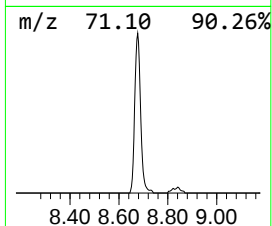
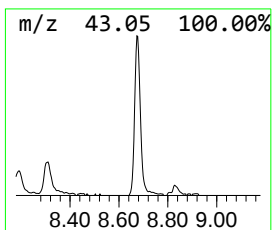
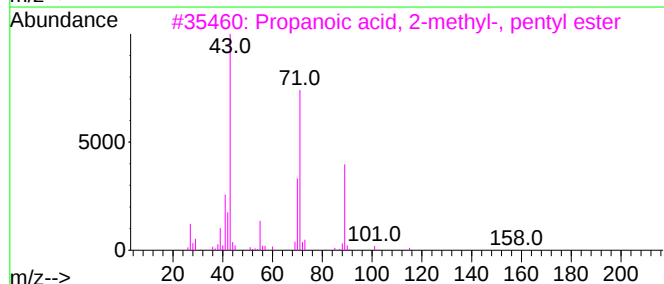
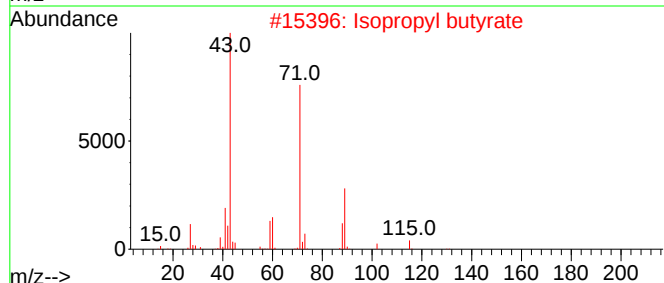
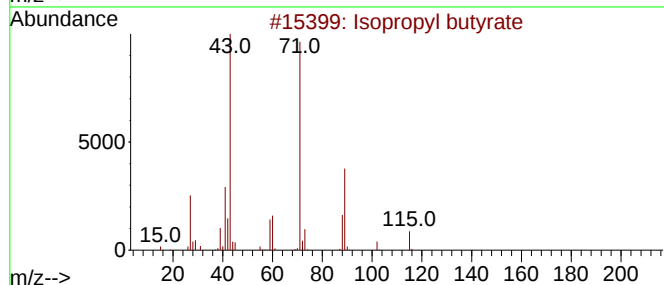
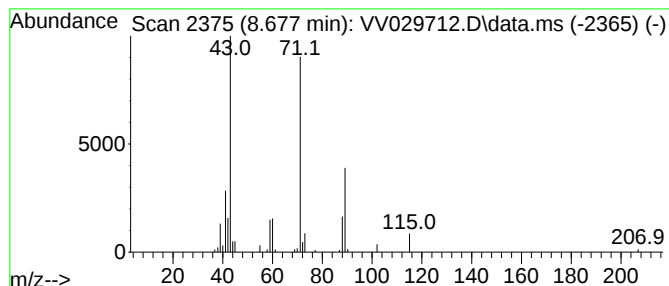
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.677	2.78 ug/L	72736	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-, penty...	158	C9H18O2	002445-72-9	72
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	72



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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.465	4.3	ug/L	93611	1	5.609	1093630	50.0
Isopropyl butyrate	8.677	2.8	ug/L	72736	2	8.844	1308680	50.0