

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV110623\
 Data File : VV032852.D
 Acq On : 06 Nov 2023 14:29
 Operator : SY/MD
 Sample : 05203-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 COAN8

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\SFAMVLM103123WMA.M
 Title : VOC Analysis

Signal : TIC: VV032852.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	68	74	88	rBV	152172	169702	12.60%	1.615%
2	2.053	306	315	329	rBV	321476	455739	33.84%	4.338%
3	2.410	421	426	428	rBV6	1184	1104	0.08%	0.011%
4	2.442	430	436	450	rVB4	7448	12896	0.96%	0.123%
5	2.625	491	493	495	rBV3	1310	742	0.06%	0.007%
6	2.648	495	500	504	rBV7	1450	1643	0.12%	0.016%
7	2.812	549	551	552	rBV	1257	466	0.03%	0.004%
8	2.825	552	555	561	rVB8	1396	1557	0.12%	0.015%
9	2.902	576	579	582	rBV5	2208	1098	0.08%	0.010%
10	2.918	582	584	585	rBV2	1205	386	0.03%	0.004%
11	2.969	598	600	602	rBV3	1388	786	0.06%	0.007%
12	2.986	602	605	607	rVV4	1554	1097	0.08%	0.010%
13	3.056	625	627	629	rBV3	1203	550	0.04%	0.005%
14	3.108	641	643	647	rBV4	2514	1542	0.11%	0.015%
15	3.201	669	672	675	rBV4	1531	959	0.07%	0.009%
16	3.224	675	679	680	rBV4	1011	724	0.05%	0.007%
17	3.259	688	690	692	rVB3	1552	614	0.05%	0.006%
18	3.285	692	698	700	rBV6	1837	1737	0.13%	0.017%
19	3.301	700	703	705	rVB3	1838	865	0.06%	0.008%
20	3.426	741	742	744	rBV	925	520	0.04%	0.005%
21	3.458	750	752	755	rBV3	1799	878	0.07%	0.008%
22	3.484	757	760	761	rBV3	909	358	0.03%	0.003%
23	3.500	763	765	767	rBV2	1247	639	0.05%	0.006%
24	3.539	776	777	780	rBV3	687	294	0.02%	0.003%
25	3.584	789	791	793	rBV3	1763	788	0.06%	0.008%
26	3.609	797	799	800	rBV2	1405	398	0.03%	0.004%
27	3.677	817	820	822	rBV4	929	498	0.04%	0.005%
28	3.725	833	835	840	rBV5	1086	682	0.05%	0.006%
29	3.786	846	854	889	rBV	75463	222647	16.53%	2.119%
30	4.249	984	998	1019	rBV	210850	547546	40.66%	5.212%
31	4.526	1081	1084	1085	rBV2	1517	815	0.06%	0.008%
32	4.658	1121	1125	1127	rBV4	1569	1032	0.08%	0.010%
33	4.828	1173	1178	1180	rVB4	1346	1065	0.08%	0.010%
34	4.841	1180	1182	1183	rBV2	786	299	0.02%	0.003%
35	4.953	1202	1217	1252	rBV2	488983	1346731	100.00%	12.818%
36	5.532	1386	1397	1428	rBV	378577	822451	61.07%	7.828%

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Integrator: RTE

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Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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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\SFAMVLM103123WMA.M
 Title : VOC Analysis

37	5.989	1528	1539	1566	rBV	287971	602056	44.70%	5.730%
38	6.400	1660	1667	1684	rBV	51980	106499	7.91%	1.014%
39	6.915	1817	1827	1849	rBV	155433	297510	22.09%	2.832%
40	7.243	1919	1929	1953	rBV	564801	1020935	75.81%	9.717%
41	7.555	2017	2026	2053	rBV2	119906	230781	17.14%	2.197%
42	7.866	2114	2123	2136	rBV	25233	47374	3.52%	0.451%
43	8.027	2164	2173	2200	rBV	294875	588632	43.71%	5.603%
44	8.593	2346	2349	2350	rBV3	2738	1554	0.12%	0.015%
45	8.622	2350	2358	2377	rVV2	61919	105249	7.82%	1.002%
46	8.744	2394	2396	2398	rBV2	1928	1180	0.09%	0.011%
47	8.786	2399	2409	2430	rVV	641935	1066664	79.20%	10.153%
48	9.403	2597	2601	2603	rBV4	1675	1350	0.10%	0.013%
49	9.612	2664	2666	2670	rVB5	1657	918	0.07%	0.009%
50	9.786	2717	2720	2721	rBV3	1654	895	0.07%	0.009%
51	9.882	2747	2750	2753	rBV5	2026	1327	0.10%	0.013%
52	10.066	2805	2807	2810	rBV3	1447	766	0.06%	0.007%
53	10.156	2823	2835	2855	rBV	445403	708850	52.63%	6.747%
54	10.564	2958	2962	2963	rBV5	1425	1049	0.08%	0.010%
55	10.603	2973	2974	2976	rBV2	1160	541	0.04%	0.005%
56	10.625	2979	2981	2986	rVV6	1542	1426	0.11%	0.014%
57	10.725	3010	3012	3013	rBV2	1733	771	0.06%	0.007%
58	10.844	3046	3049	3050	rBV3	1684	749	0.06%	0.007%
59	11.017	3099	3103	3105	rBV5	1889	1336	0.10%	0.013%
60	11.120	3130	3135	3138	rBV7	1843	2381	0.18%	0.023%
61	11.188	3144	3156	3176	rBV	647704	1007596	74.82%	9.590%
62	11.480	3245	3247	3248	rBV2	1408	426	0.03%	0.004%
63	11.564	3260	3273	3290	rBV	684216	1087172	80.73%	10.348%
64	11.943	3388	3391	3393	rBV3	1169	831	0.06%	0.008%
65	12.005	3408	3410	3412	rBV3	1381	713	0.05%	0.007%
66	12.213	3471	3475	3481	rBV7	1691	2265	0.17%	0.022%
67	12.259	3486	3489	3490	rBV2	1113	568	0.04%	0.005%
68	12.294	3496	3500	3505	rBV8	2095	1880	0.14%	0.018%
69	12.429	3540	3542	3545	rBV4	1406	671	0.05%	0.006%
70	12.529	3569	3573	3576	rBV6	1247	981	0.07%	0.009%
71	12.754	3641	3643	3648	rVB5	2160	1658	0.12%	0.016%
72	12.866	3676	3678	3681	rBV3	1094	632	0.05%	0.006%
73	12.914	3690	3693	3698	rBV6	1886	1997	0.15%	0.019%
74	12.963	3705	3708	3710	rBV4	1184	596	0.04%	0.006%
75	13.516	3878	3880	3883	rBV4	1579	755	0.06%	0.007%
76	13.580	3898	3900	3902	rBV3	1078	641	0.05%	0.006%

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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\SFAMVLM103123WMA.M
Title : VOC Analysis

77	13.612	3907	3910	3913	rBV5	2294	1550	0.12%	0.015%
78	14.078	4052	4055	4056	rBV3	1749	858	0.06%	0.008%
79	14.493	4181	4184	4188	rBV6	1933	1826	0.14%	0.017%

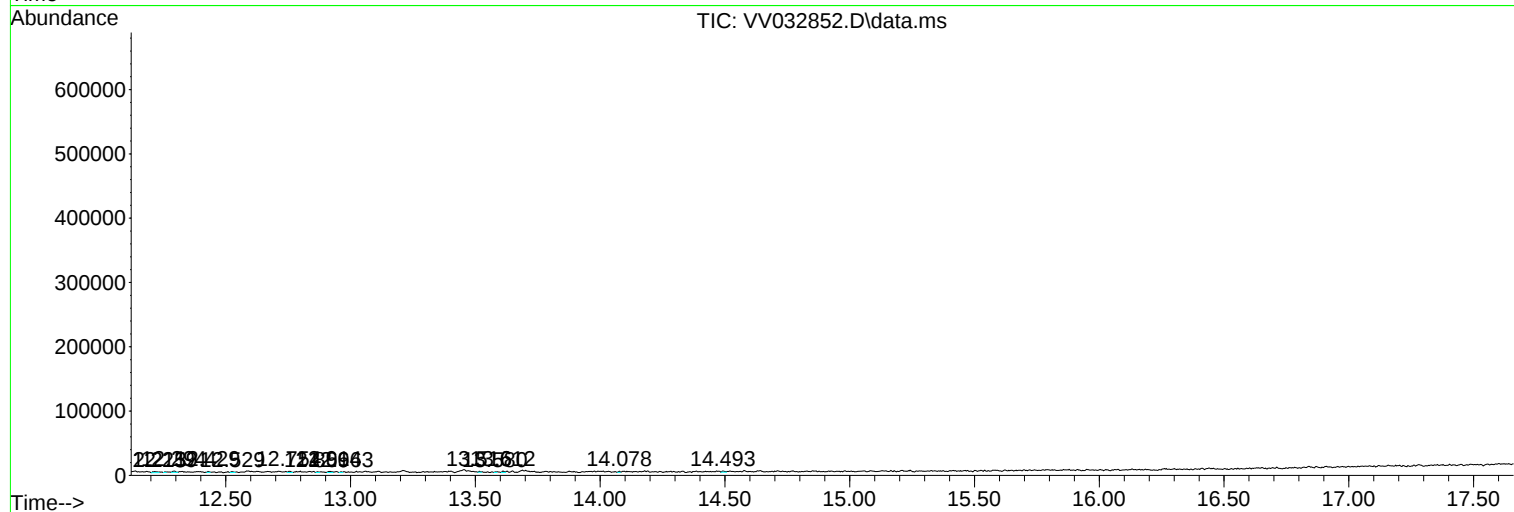
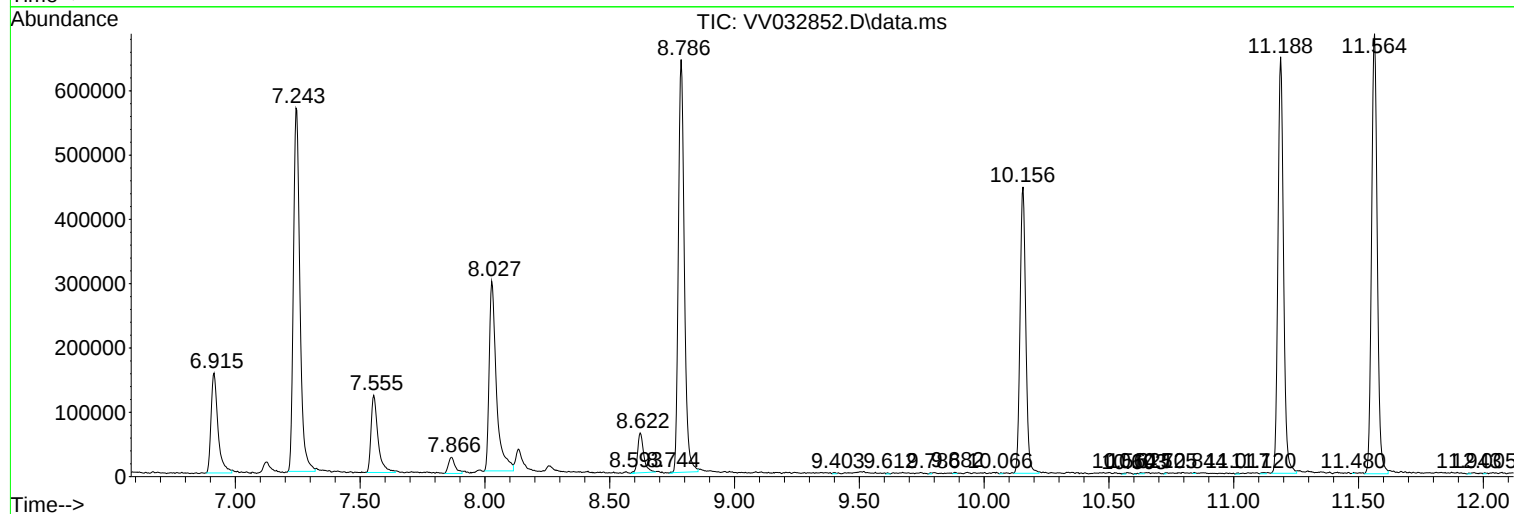
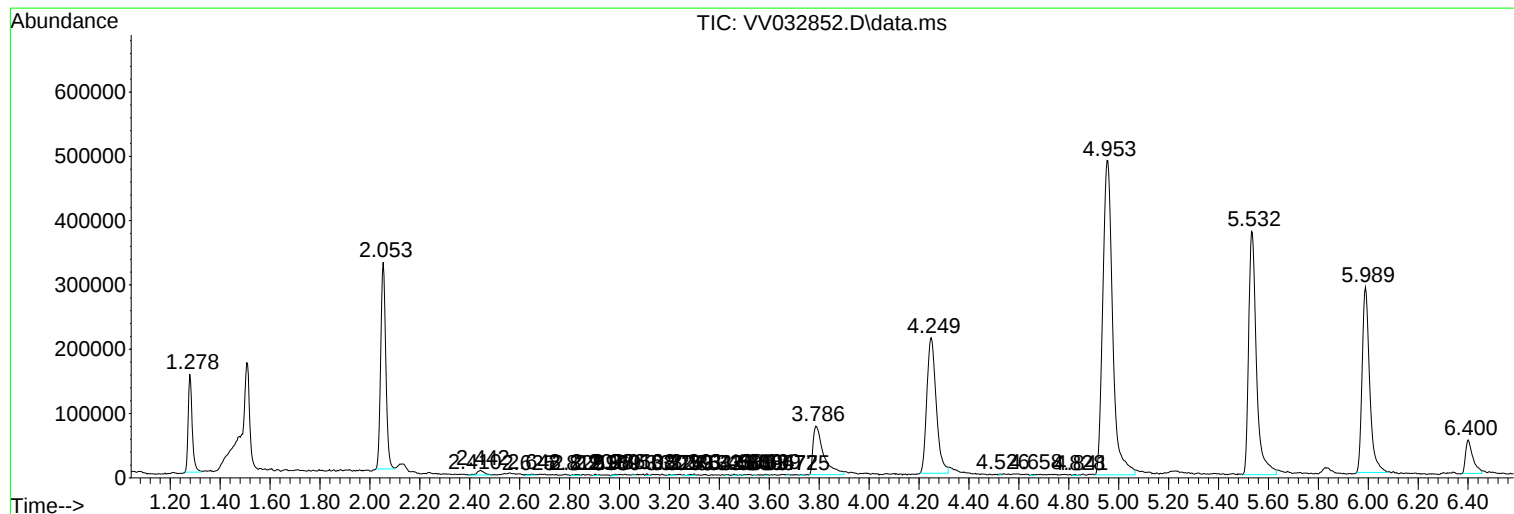
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM103123WMA.M
Quant Title : VOC Analysis

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



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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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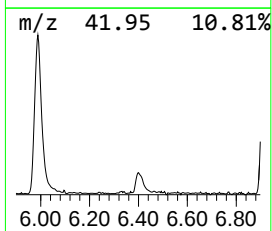
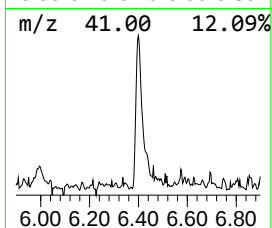
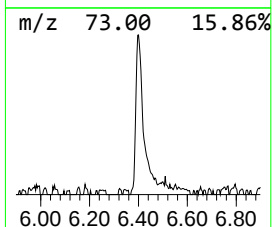
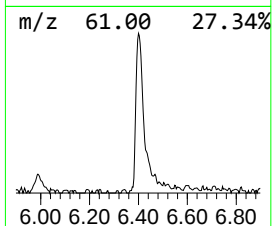
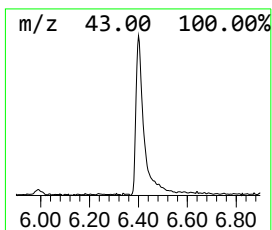
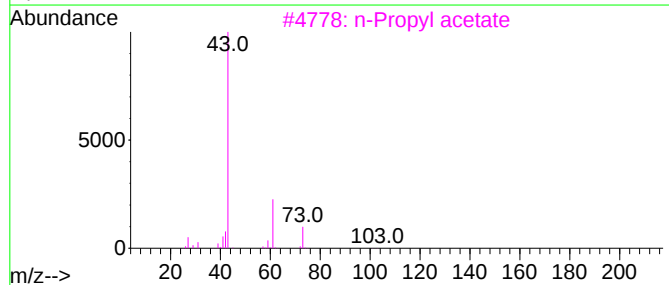
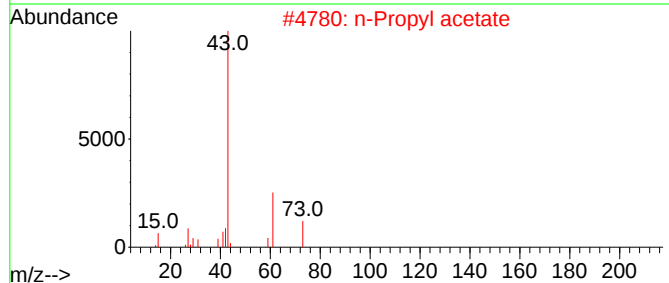
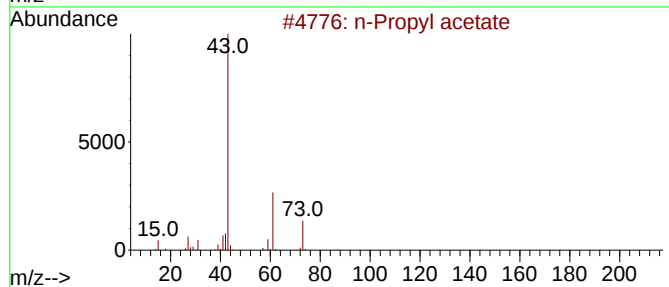
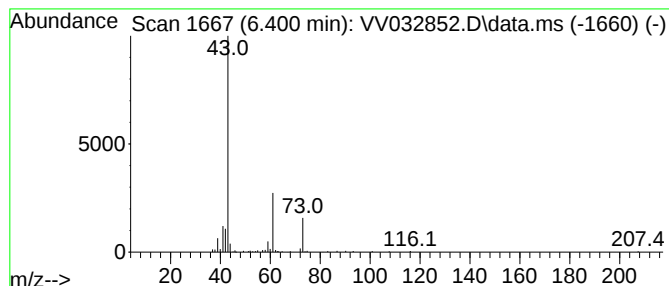
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM103123WMA.M
Quant Title : VOC Analysis

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.
6.400	6.47 ug/L	106499	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	78
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	59



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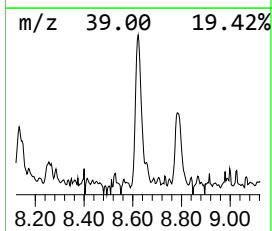
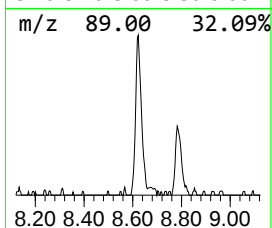
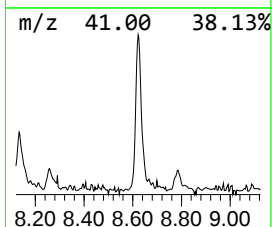
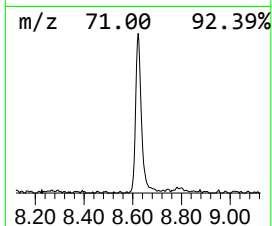
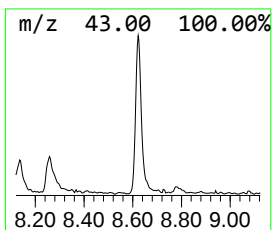
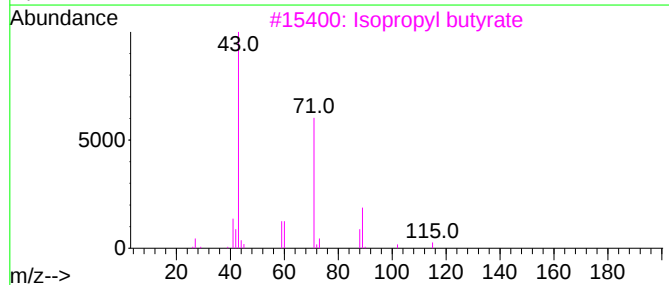
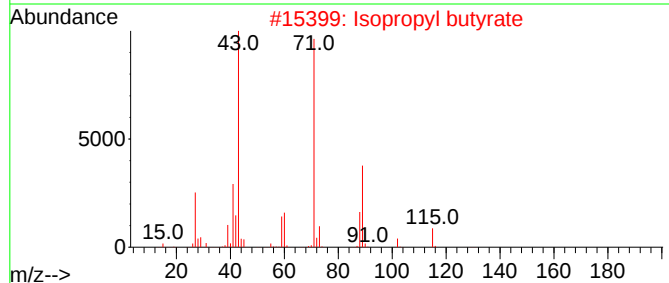
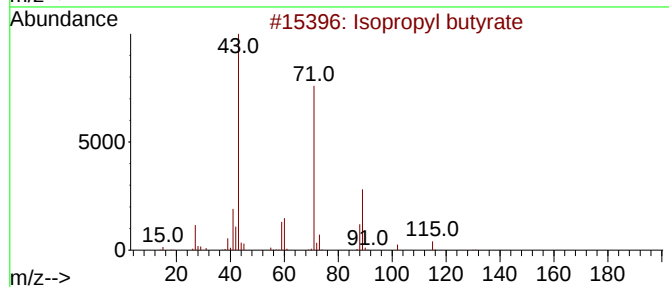
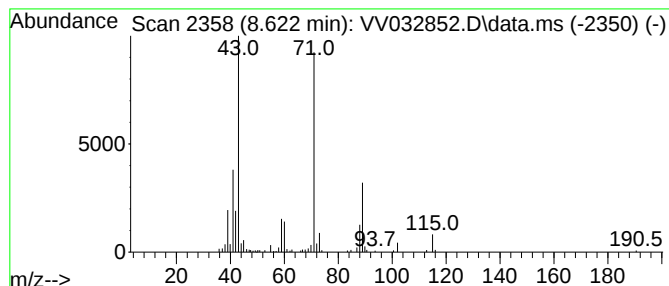
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM103123WMA.M
Quant Title : VOC Analysis

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.
8.622	4.93 ug/L	105249	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	86
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	86
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64



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C0AN8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM103123WMA.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	6.400	6.5	ug/L	106499	1	5.535	822451	50.0
Isopropyl butyrate	8.622	4.9	ug/L	105249	2	8.786	1066660	50.0