

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
 Data File : VV033329.D
 Acq On : 14 Dec 2023 12:54
 Operator : SY/MD
 Sample : 05682-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCLD6

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\SFAMVLM120123WMA.M
 Title : VOC Analysis

Signal : TIC: VV033329.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	69	74	93	rVB	106922	113506	13.25%	1.748%
2	1.532	147	153	166	rVB	78767	90944	10.62%	1.400%
3	2.060	308	317	328	rBV	173740	249085	29.08%	3.835%
4	2.346	403	406	409	rBV	290	180	0.02%	0.003%
5	2.384	415	418	422	rBB2	405	276	0.03%	0.004%
6	2.404	423	424	429	rBV	335	258	0.03%	0.004%
7	2.449	429	438	449	rVB3	7799	13339	1.56%	0.205%
8	2.561	470	473	480	rBV3	687	773	0.09%	0.012%
9	2.648	497	500	501	rBV	237	136	0.02%	0.002%
10	2.680	506	510	514	rBV2	279	330	0.04%	0.005%
11	2.728	523	525	532	rVB	385	394	0.05%	0.006%
12	2.773	533	539	542	rBB2	278	335	0.04%	0.005%
13	2.789	542	544	546	rBV	244	132	0.02%	0.002%
14	3.047	622	624	629	rBV2	290	271	0.03%	0.004%
15	3.114	642	645	648	rBB	148	119	0.01%	0.002%
16	3.252	684	688	690	rBV	179	158	0.02%	0.002%
17	3.301	701	703	707	rBV	157	150	0.02%	0.002%
18	3.339	712	715	717	rBV	144	127	0.01%	0.002%
19	3.442	744	747	750	rBV	323	260	0.03%	0.004%
20	3.481	755	759	762	rBB	172	158	0.02%	0.002%
21	3.506	763	767	768	rBV	222	111	0.01%	0.002%
22	3.558	781	783	789	rBB	173	189	0.02%	0.003%
23	3.603	794	797	800	rBB	178	133	0.02%	0.002%
24	3.719	831	833	836	rBB	363	212	0.02%	0.003%
25	3.783	844	853	886	rBV	39880	110535	12.91%	1.702%
26	4.249	982	998	1025	rBV2	143003	366739	42.82%	5.647%
27	4.535	1084	1087	1088	rBV	182	119	0.01%	0.002%
28	4.654	1122	1124	1126	rVB2	548	268	0.03%	0.004%
29	4.725	1142	1146	1147	rBV	294	173	0.02%	0.003%
30	4.770	1157	1160	1161	rBV	165	118	0.01%	0.002%
31	4.841	1180	1182	1184	rBV	168	120	0.01%	0.002%
32	4.892	1196	1198	1201	rBV	278	219	0.03%	0.003%
33	4.957	1201	1218	1247	rBV2	322921	856513	100.00%	13.188%
34	5.532	1386	1397	1424	rBV	260295	533564	62.29%	8.216%
35	5.989	1526	1539	1574	rBV	177245	366336	42.77%	5.641%
36	6.284	1623	1631	1644	rBV2	2418	6288	0.73%	0.097%

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37	6.593	1722	1727	1730	rBB3	607	451	0.05%	0.007%
38	6.628	1733	1738	1741	rBV3	389	340	0.04%	0.005%
39	6.744	1771	1774	1775	rBV	257	127	0.01%	0.002%
40	6.805	1790	1793	1795	rBV	137	115	0.01%	0.002%
41	6.841	1802	1804	1807	rBV	133	122	0.01%	0.002%
42	6.911	1816	1826	1847	rBV	102001	191054	22.31%	2.942%
43	7.243	1918	1929	1955	rBV	409825	723989	84.53%	11.148%
44	7.551	2016	2025	2055	rBV	74586	134690	15.73%	2.074%
45	7.863	2108	2122	2137	rBV2	23128	42264	4.93%	0.651%
46	7.953	2145	2150	2152	rBV3	1716	1608	0.19%	0.025%
47	8.435	2296	2300	2302	rBV2	464	326	0.04%	0.005%
48	8.455	2305	2306	2309	rVB	360	179	0.02%	0.003%
49	8.481	2310	2314	2316	rBV	367	210	0.02%	0.003%
50	8.583	2343	2346	2347	rBV2	384	213	0.02%	0.003%
51	8.622	2348	2358	2374	rVV3	24621	44059	5.14%	0.678%
52	8.728	2390	2391	2394	rVB	446	143	0.02%	0.002%
53	8.786	2398	2409	2428	rBV	418764	694198	81.05%	10.689%
54	8.998	2474	2475	2477	rVB2	367	138	0.02%	0.002%
55	9.101	2503	2507	2510	rBV	265	256	0.03%	0.004%
56	9.120	2510	2513	2517	rVB3	448	372	0.04%	0.006%
57	9.146	2517	2521	2523	rBV2	272	201	0.02%	0.003%
58	9.220	2540	2544	2546	rBV	246	250	0.03%	0.004%
59	9.262	2555	2557	2559	rBB	241	134	0.02%	0.002%
60	9.291	2565	2566	2569	rBV	226	125	0.01%	0.002%
61	9.307	2569	2571	2574	rVB	269	125	0.01%	0.002%
62	9.419	2604	2606	2608	rBV	378	235	0.03%	0.004%
63	9.477	2621	2624	2625	rBV	219	130	0.02%	0.002%
64	9.593	2655	2660	2664	rBB2	334	331	0.04%	0.005%
65	9.654	2677	2679	2682	rBB2	217	125	0.01%	0.002%
66	9.786	2717	2720	2722	rBV2	353	263	0.03%	0.004%
67	9.850	2737	2740	2744	rBV	292	338	0.04%	0.005%
68	9.963	2773	2775	2777	rBB	226	105	0.01%	0.002%
69	9.982	2778	2781	2784	rBV	170	158	0.02%	0.002%
70	10.050	2799	2802	2808	rBB2	353	301	0.04%	0.005%
71	10.075	2808	2810	2814	rBB	324	216	0.03%	0.003%
72	10.152	2823	2834	2859	rVV2	272807	428078	49.98%	6.591%
73	10.268	2866	2870	2874	rBV2	437	405	0.05%	0.006%
74	10.590	2966	2970	2973	rBV2	368	316	0.04%	0.005%
75	10.664	2990	2993	2996	rBB	206	153	0.02%	0.002%
76	10.693	2999	3002	3003	rBV	180	123	0.01%	0.002%

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 Title : VOC Analysis

77	10.767	3023	3025	3027	rBV	243	180	0.02%	0.003%
78	10.892	3062	3064	3066	rBV	281	173	0.02%	0.003%
79	10.940	3076	3079	3085	rVB2	325	348	0.04%	0.005%
80	10.969	3085	3088	3091	rBB	141	117	0.01%	0.002%
81	10.995	3092	3096	3098	rBV	327	248	0.03%	0.004%
82	11.030	3105	3107	3112	rBV2	303	305	0.04%	0.005%
83	11.082	3117	3123	3125	rBV2	276	287	0.03%	0.004%
84	11.185	3144	3155	3184	rBV	454452	729716	85.20%	11.236%
85	11.561	3260	3272	3290	rBV	490513	779659	91.03%	12.005%
86	11.767	3330	3336	3337	rBV2	433	432	0.05%	0.007%
87	11.927	3383	3386	3389	rBB2	278	209	0.02%	0.003%
88	12.043	3419	3422	3424	rBV	165	146	0.02%	0.002%
89	12.320	3506	3508	3509	rBV	231	113	0.01%	0.002%
90	12.410	3533	3536	3537	rBV	257	149	0.02%	0.002%
91	12.439	3542	3545	3548	rBV2	233	175	0.02%	0.003%
92	12.487	3557	3560	3563	rBV	227	151	0.02%	0.002%
93	12.593	3588	3593	3597	rBV3	785	752	0.09%	0.012%
94	12.847	3670	3672	3677	rBV	226	145	0.02%	0.002%
95	12.898	3680	3688	3691	rBV2	393	489	0.06%	0.008%
96	12.950	3700	3704	3706	rBB	382	266	0.03%	0.004%
97	12.966	3706	3709	3711	rBV	173	146	0.02%	0.002%
98	13.082	3743	3745	3747	rBV	247	164	0.02%	0.003%
99	13.191	3775	3779	3780	rBV2	402	254	0.03%	0.004%
100	13.590	3899	3903	3905	rBV2	392	363	0.04%	0.006%

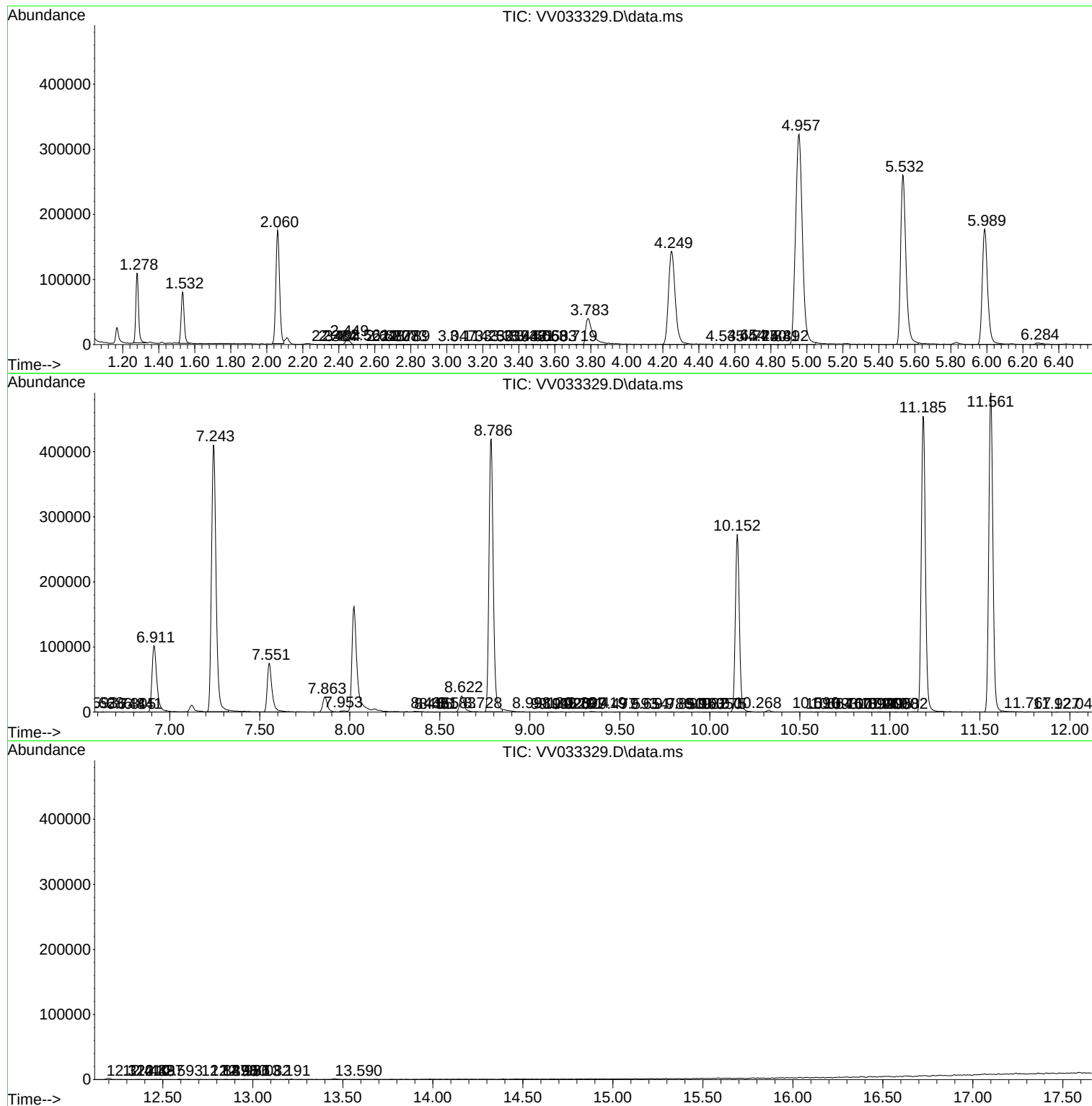
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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



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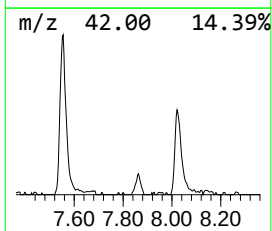
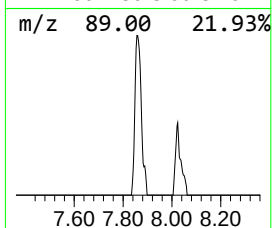
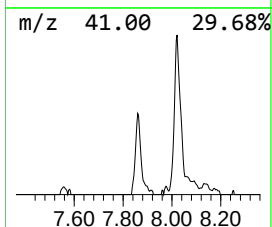
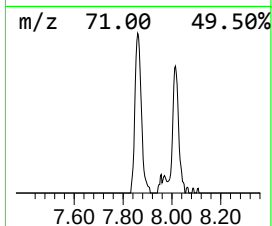
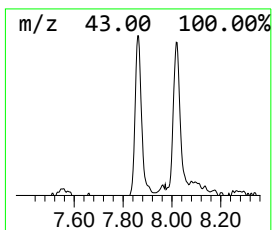
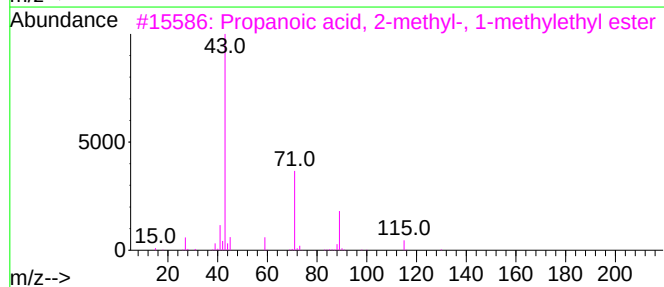
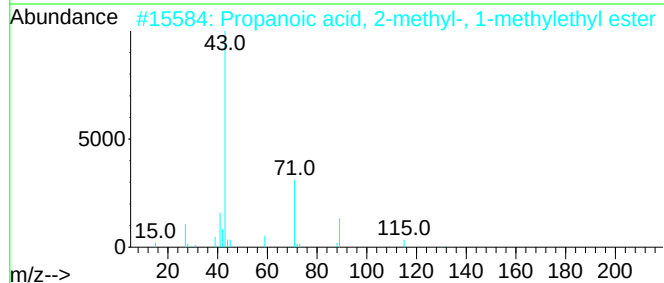
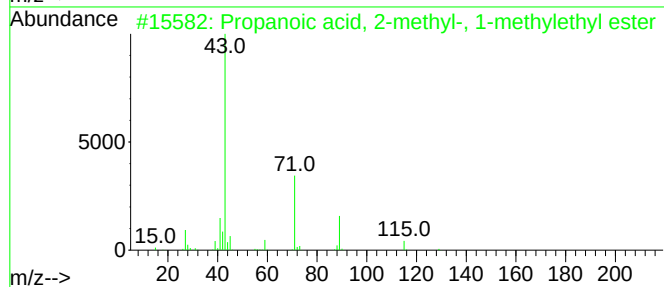
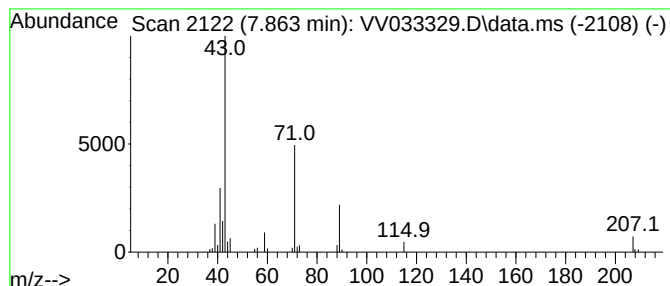
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	3.04 ug/L	42264	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	78
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	72
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	64
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64



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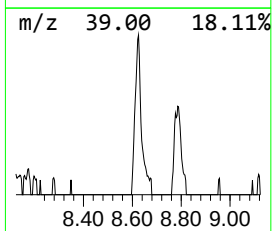
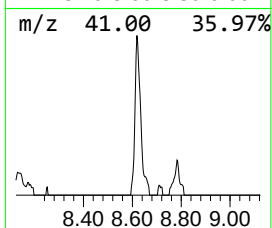
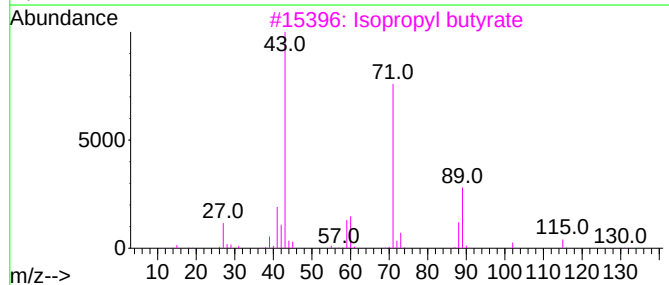
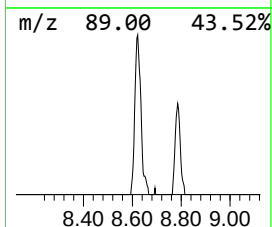
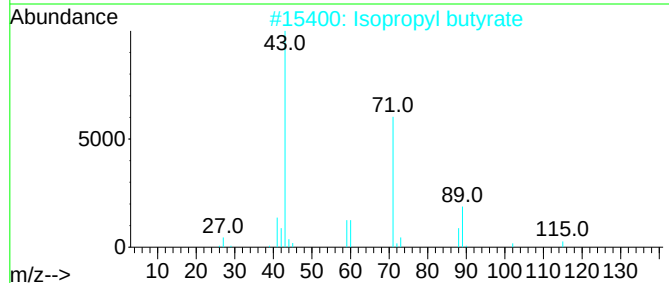
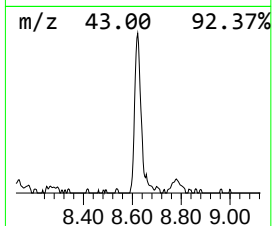
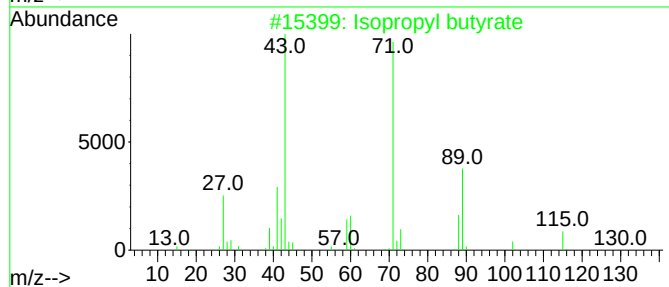
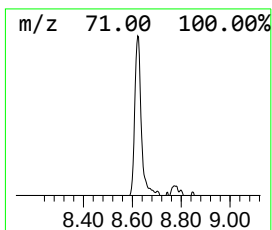
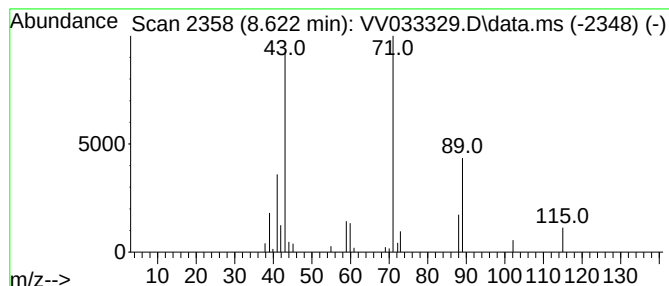
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.622	3.17 ug/L	44059	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	83
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	64



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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
Propanoic acid,...	7.863	3.0	ug/L	42264	2	8.786	694198	50.0
Isopropyl butyrate	8.622	3.2	ug/L	44059	2	8.786	694198	50.0