

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
 Data File : VU055773.D
 Acq On : 16 Oct 2023 15:37
 Operator : MD/SY
 Sample : 04852-01 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DCJV3

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_U\Method\SFAMULM101023WMA.M

Title : VOC Analysis

Signal : TIC: VU055773.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	88	96	112	rBV	220314	260526	14.14%	1.792%
2	1.891	180	187	205	rVB	179930	255677	13.88%	1.758%
3	2.560	383	395	410	rBV	371506	605188	32.86%	4.162%
4	2.991	527	529	531	rBV2	300	146	0.01%	0.001%
5	3.039	534	544	559	rVB2	10540	19935	1.08%	0.137%
6	3.123	567	570	572	rBV	174	132	0.01%	0.001%
7	3.133	572	573	575	rVB	353	126	0.01%	0.001%
8	3.181	575	588	600	rBV2	4236	9518	0.52%	0.065%
9	3.293	619	623	625	rBV2	250	208	0.01%	0.001%
10	3.338	633	637	640	rBV	355	270	0.01%	0.002%
11	3.428	663	665	666	rBV	323	83	0.00%	0.001%
12	3.441	666	669	671	rVB2	249	148	0.01%	0.001%
13	3.457	671	674	681	rVB2	282	290	0.02%	0.002%
14	3.486	681	683	685	rBV	132	66	0.00%	0.000%
15	3.506	685	689	690	rBV	194	139	0.01%	0.001%
16	3.541	698	700	704	rBV3	225	185	0.01%	0.001%
17	3.573	708	710	711	rBV3	242	86	0.00%	0.001%
18	3.715	753	754	757	rVB	275	103	0.01%	0.001%
19	3.734	757	760	764	rBV	436	343	0.02%	0.002%
20	3.766	768	770	771	rBV	271	122	0.01%	0.001%
21	3.785	774	776	781	rVB2	201	149	0.01%	0.001%
22	3.811	781	784	786	rBV	227	130	0.01%	0.001%
23	3.862	798	800	803	rVB	305	110	0.01%	0.001%
24	3.888	805	808	810	rBV	188	98	0.01%	0.001%
25	3.920	815	818	822	rBV	245	190	0.01%	0.001%
26	3.975	830	835	840	rBV	375	369	0.02%	0.003%
27	4.078	862	867	870	rVV2	251	227	0.01%	0.002%
28	4.097	870	873	876	rVB2	459	274	0.01%	0.002%
29	4.123	876	881	884	rBV	149	126	0.01%	0.001%
30	4.142	884	887	892	rVB2	402	263	0.01%	0.002%
31	4.168	892	895	897	rVB	120	64	0.00%	0.000%
32	4.190	899	902	905	rBV	457	262	0.01%	0.002%
33	4.251	917	921	926	rBV3	434	423	0.02%	0.003%
34	4.290	931	933	934	rBV	212	114	0.01%	0.001%
35	4.338	942	948	951	rBV3	326	310	0.02%	0.002%
36	4.386	958	963	966	rBV3	418	338	0.02%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

37	4.415	969	972	975	rBV2	284	186	0.01%	0.001%
38	4.534	1007	1009	1012	rVB	197	112	0.01%	0.001%
39	4.557	1014	1016	1018	rBV	148	65	0.00%	0.000%
40	4.570	1018	1020	1023	rVB2	176	77	0.00%	0.001%
41	4.615	1023	1034	1062	rBV	129284	341972	18.57%	2.352%
42	5.055	1155	1171	1193	rBV	339753	752849	40.87%	5.178%
43	5.316	1249	1252	1254	rBV3	645	466	0.03%	0.003%
44	5.399	1273	1278	1283	rVB3	482	506	0.03%	0.003%
45	5.460	1289	1297	1304	rVB2	364	534	0.03%	0.004%
46	5.496	1304	1308	1309	rBV	264	133	0.01%	0.001%
47	5.534	1317	1320	1321	rBV	315	136	0.01%	0.001%
48	5.567	1325	1330	1334	rVB2	411	443	0.02%	0.003%
49	5.586	1334	1336	1338	rBV2	183	100	0.01%	0.001%
50	5.602	1338	1341	1342	rBV	209	113	0.01%	0.001%
51	5.628	1347	1349	1351	rBV	165	104	0.01%	0.001%
52	5.640	1351	1353	1357	rVB	263	155	0.01%	0.001%
53	5.718	1357	1377	1402	rBV2	672625	1841966	100.00%	12.668%
54	6.100	1493	1496	1499	rVB3	423	264	0.01%	0.002%
55	6.155	1511	1513	1518	rVB4	468	381	0.02%	0.003%
56	6.194	1523	1525	1526	rBV	262	77	0.00%	0.001%
57	6.242	1527	1540	1559	rBV	528840	1017268	55.23%	6.996%
58	6.531	1617	1630	1642	rBV3	18425	36061	1.96%	0.248%
59	6.685	1662	1678	1708	rBV	434158	870270	47.25%	5.985%
60	6.888	1739	1741	1744	rVB2	397	157	0.01%	0.001%
61	6.930	1744	1754	1771	rBV	6844	16967	0.92%	0.117%
62	7.036	1777	1787	1807	rBV	129296	237663	12.90%	1.635%
63	7.319	1871	1875	1877	rBV3	477	324	0.02%	0.002%
64	7.560	1938	1950	1974	rBV2	224570	407911	22.15%	2.805%
65	7.737	1997	2005	2016	rVB	27986	47349	2.57%	0.326%
66	7.894	2041	2054	2083	rBV	835828	1467278	79.66%	10.091%
67	8.174	2126	2141	2170	rBV2	171582	339501	18.43%	2.335%
68	8.341	2191	2193	2197	rVB2	674	427	0.02%	0.003%
69	8.464	2218	2231	2243	rBV	38544	65086	3.53%	0.448%
70	8.634	2272	2284	2306	rBV4	338878	821192	44.58%	5.648%
71	8.836	2339	2347	2362	rVB	33774	57283	3.11%	0.394%
72	9.036	2405	2409	2411	rBV2	508	405	0.02%	0.003%
73	9.110	2430	2432	2435	rVB	439	252	0.01%	0.002%
74	9.152	2443	2445	2446	rBV	232	98	0.01%	0.001%
75	9.164	2447	2449	2451	rVV2	636	304	0.02%	0.002%
76	9.209	2451	2463	2484	rVV2	100320	170986	9.28%	1.176%

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 Title : VOC Analysis

77	9.415	2514	2527	2549	rBV	771450	1310930	71.17%	9.016%
78	9.627	2589	2593	2594	rBV3	642	535	0.03%	0.004%
79	9.669	2604	2606	2610	rVB2	918	507	0.03%	0.003%
80	9.701	2610	2616	2620	rBV5	1312	1208	0.07%	0.008%
81	9.872	2666	2669	2673	rVB2	464	374	0.02%	0.003%
82	9.891	2673	2675	2677	rBV	196	94	0.01%	0.001%
83	9.917	2680	2683	2684	rBV3	641	390	0.02%	0.003%
84	10.010	2710	2712	2718	rBB2	323	238	0.01%	0.002%
85	10.078	2725	2733	2742	rBV4	5354	9022	0.49%	0.062%
86	10.180	2763	2765	2766	rBV	272	101	0.01%	0.001%
87	10.216	2774	2776	2779	rVB2	342	134	0.01%	0.001%
88	10.258	2786	2789	2791	rBV2	334	245	0.01%	0.002%
89	10.753	2930	2943	2967	rBV	624773	1024064	55.60%	7.043%
90	10.968	3008	3010	3011	rBB	121	99	0.01%	0.001%
91	11.023	3021	3027	3030	rBV2	453	365	0.02%	0.003%
92	11.049	3030	3035	3038	rBV	425	320	0.02%	0.002%
93	11.123	3055	3058	3061	rBV	362	216	0.01%	0.001%
94	11.274	3102	3105	3107	rBV2	367	253	0.01%	0.002%
95	11.615	3208	3211	3212	rBV2	329	174	0.01%	0.001%
96	11.811	3259	3272	3295	rBV	730787	1192515	64.74%	8.201%
97	12.190	3377	3390	3414	rBV	804280	1343222	72.92%	9.238%
98	12.814	3580	3584	3586	rBV	388	314	0.02%	0.002%
99	12.846	3592	3594	3597	rBV	406	227	0.01%	0.002%
100	13.322	3738	3742	3746	rBV3	783	686	0.04%	0.005%

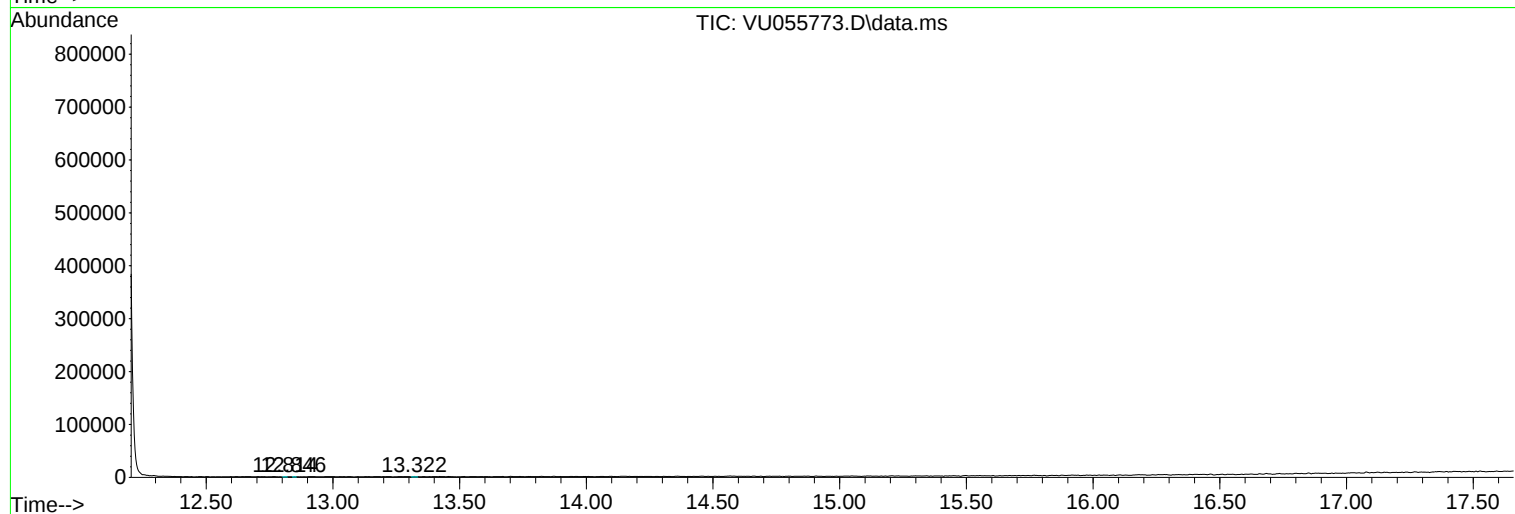
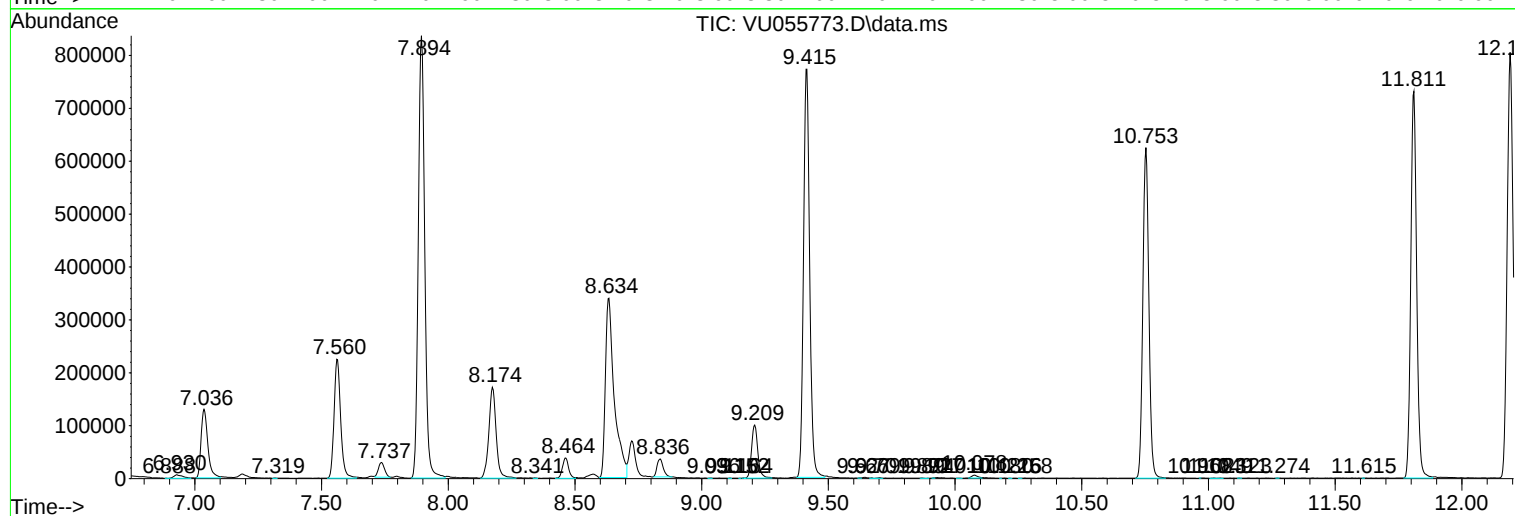
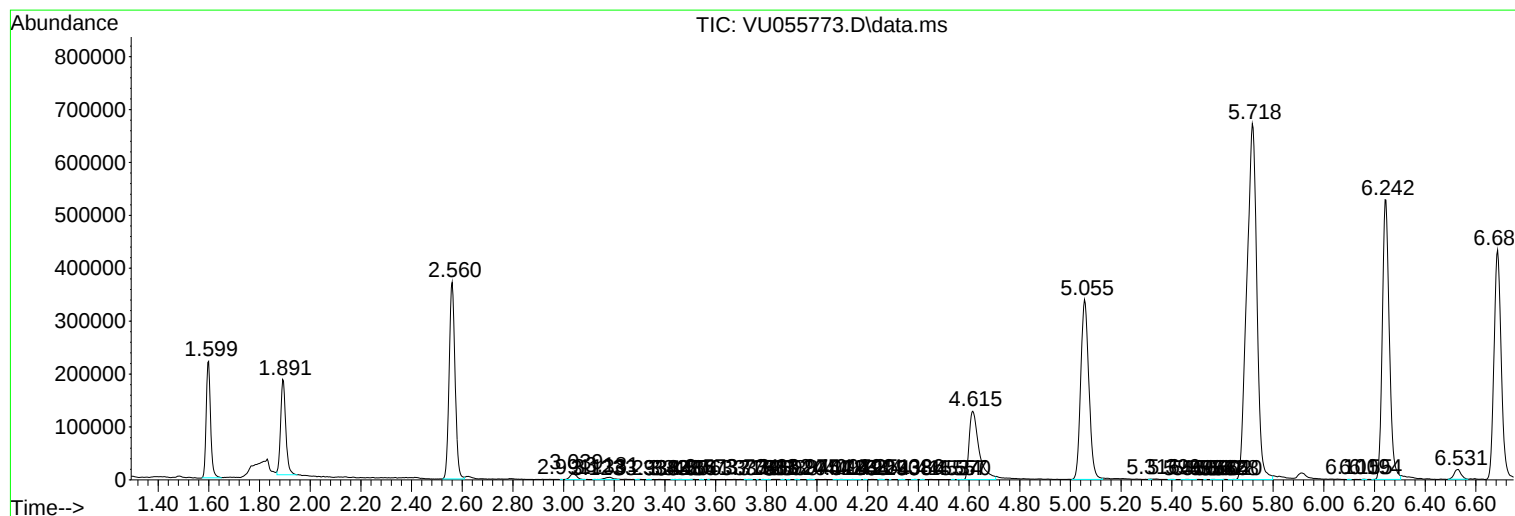
Sum of corrected areas: 14540392

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P



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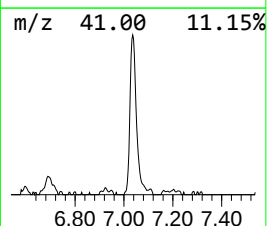
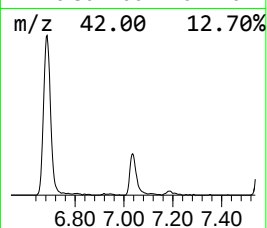
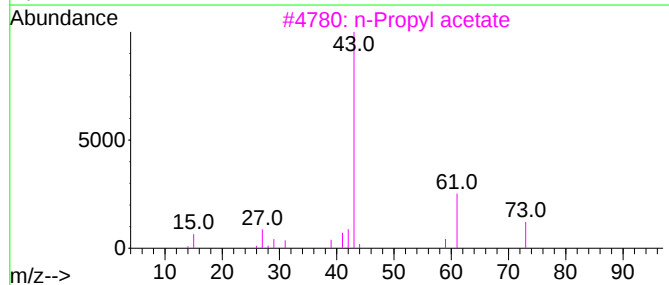
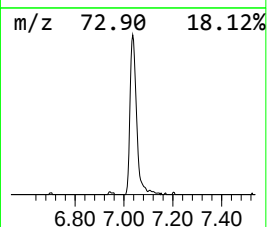
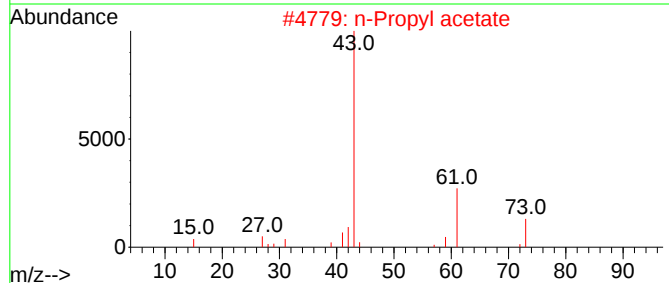
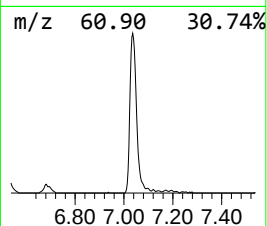
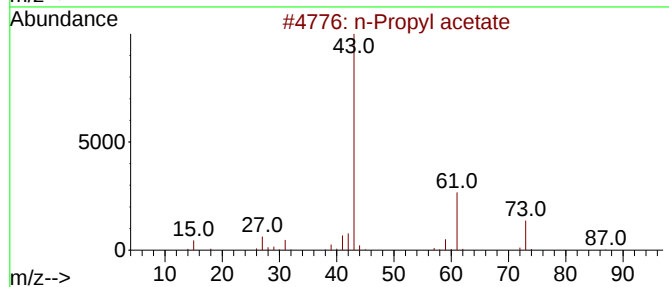
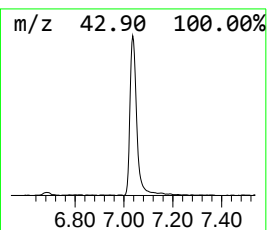
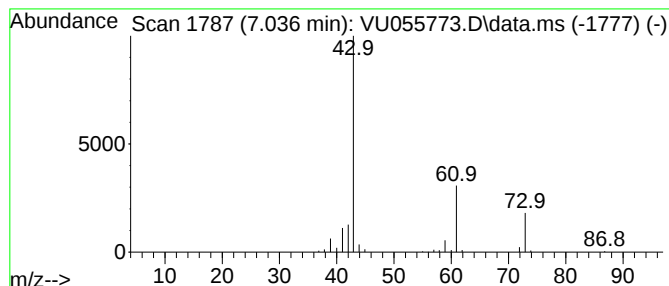
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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.
7.036	11.68 ug/L	237663	1,4-Difluorobenzene	6.245

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	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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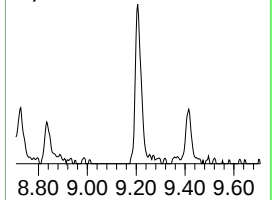
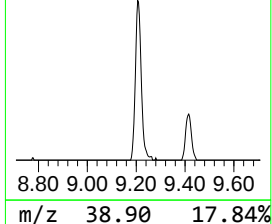
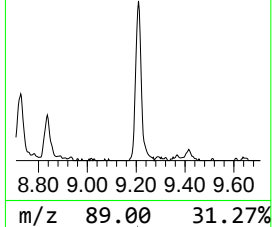
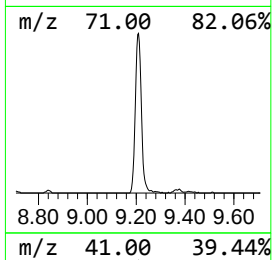
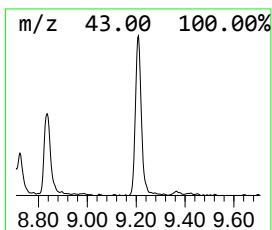
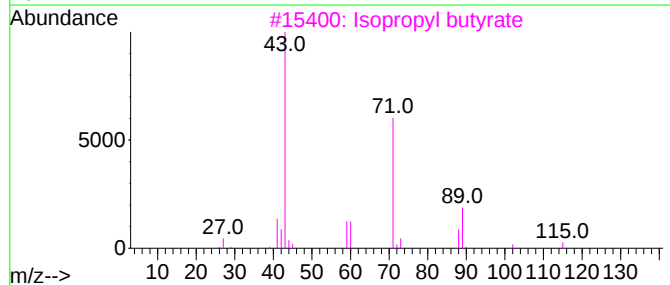
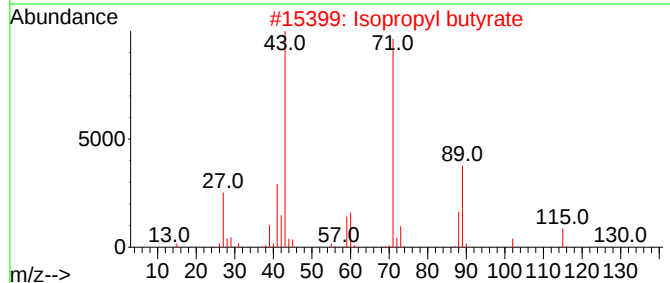
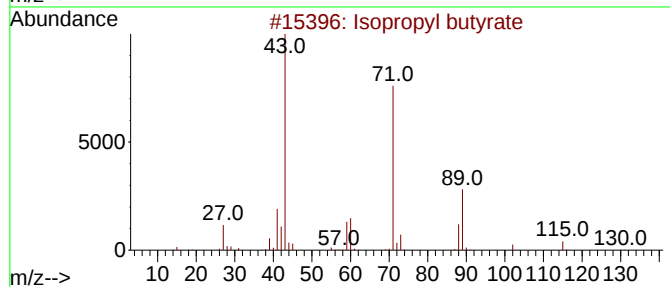
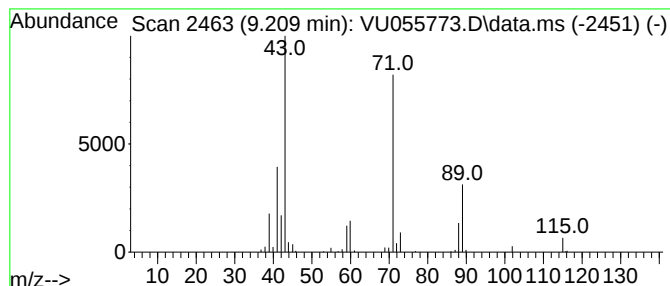
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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.
9.209	6.52 ug/L	170986	Chlorobenzene-d5	9.415

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	86
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, propyl ester	130	C7H14O2	000105-66-8	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
n-Propyl acetate	7.036	11.7	ug/L	237663	1	6.245	1017270	50.0
Isopropyl butyrate	9.209	6.5	ug/L	170986	2	9.415	1310930	50.0