

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
 Data File : VU055771.D
 Acq On : 16 Oct 2023 14:49
 Operator : MD/SY
 Sample : 04874-01 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COM25

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: VU055771.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	87	96	113	rBV	247575	297112	13.97%	1.867%
2	1.891	179	187	210	rVB	201756	302632	14.23%	1.902%
3	2.560	381	395	409	rBV	428974	708252	33.29%	4.450%
4	2.682	430	433	435	rBV2	664	408	0.02%	0.003%
5	2.859	484	488	490	rBV2	730	458	0.02%	0.003%
6	2.930	508	510	516	rVV3	452	442	0.02%	0.003%
7	3.036	533	543	556	rVB3	11283	20864	0.98%	0.131%
8	3.177	573	587	601	rBV	6474	15147	0.71%	0.095%
9	3.383	650	651	658	rVB2	444	295	0.01%	0.002%
10	3.570	705	709	716	rVV2	336	360	0.02%	0.002%
11	3.795	777	779	785	rVB2	467	356	0.02%	0.002%
12	3.849	793	796	799	rBV3	498	359	0.02%	0.002%
13	4.161	888	893	898	rBV2	323	338	0.02%	0.002%
14	4.213	904	909	912	rBV2	317	302	0.01%	0.002%
15	4.467	986	988	992	rBV2	471	367	0.02%	0.002%
16	4.496	992	997	1002	rVB2	401	441	0.02%	0.003%
17	4.525	1002	1006	1011	rBV2	380	398	0.02%	0.003%
18	4.615	1022	1034	1063	rBV2	153019	406690	19.12%	2.555%
19	4.820	1096	1098	1102	rBV4	754	460	0.02%	0.003%
20	4.911	1124	1126	1131	rBV2	609	462	0.02%	0.003%
21	4.975	1140	1146	1148	rBV3	547	526	0.02%	0.003%
22	5.055	1154	1171	1197	rBV	392976	874232	41.10%	5.493%
23	5.486	1303	1305	1310	rVB2	417	315	0.01%	0.002%
24	5.547	1320	1324	1327	rBV2	424	302	0.01%	0.002%
25	5.602	1335	1341	1346	rVB3	449	504	0.02%	0.003%
26	5.644	1351	1354	1356	rBV2	603	382	0.02%	0.002%
27	5.718	1356	1377	1402	rBV2	765884	2127254	100.00%	13.366%
28	5.910	1431	1437	1456	rVB3	8677	17041	0.80%	0.107%
29	6.010	1466	1468	1471	rVB	723	346	0.02%	0.002%
30	6.036	1471	1476	1478	rBV4	660	688	0.03%	0.004%
31	6.116	1497	1501	1503	rBV3	438	317	0.01%	0.002%
32	6.177	1518	1520	1524	rVB	461	306	0.01%	0.002%
33	6.245	1527	1541	1564	rBV	531069	1030923	48.46%	6.478%
34	6.528	1618	1629	1644	rVB2	20925	41284	1.94%	0.259%
35	6.592	1644	1649	1651	rBV4	768	623	0.03%	0.004%
36	6.685	1661	1678	1710	rBV	490459	971066	45.65%	6.102%

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 Title : VOC Analysis

37	6.930	1745	1754	1757	rBV	5918	8814	0.41%	0.055%
38	7.036	1778	1787	1808	rBV2	69436	133747	6.29%	0.840%
39	7.187	1824	1834	1845	rBV5	7081	14008	0.66%	0.088%
40	7.319	1871	1875	1879	rVB3	568	457	0.02%	0.003%
41	7.348	1881	1884	1887	rVB2	525	312	0.01%	0.002%
42	7.390	1892	1897	1901	rVV2	391	419	0.02%	0.003%
43	7.412	1901	1904	1909	rVB3	513	368	0.02%	0.002%
44	7.454	1914	1917	1919	rBV2	487	310	0.01%	0.002%
45	7.560	1937	1950	1976	rBV	252342	458392	21.55%	2.880%
46	7.698	1986	1993	1996	rBV4	2614	3604	0.17%	0.023%
47	7.737	1997	2005	2017	rVB2	25964	43658	2.05%	0.274%
48	7.788	2017	2021	2023	rBV2	1665	1342	0.06%	0.008%
49	7.894	2040	2054	2083	rBV	941623	1651867	77.65%	10.379%
50	8.174	2127	2141	2159	rBV	187809	337781	15.88%	2.122%
51	8.354	2194	2197	2199	rVV	663	324	0.02%	0.002%
52	8.373	2199	2203	2206	rVB3	452	381	0.02%	0.002%
53	8.460	2219	2230	2243	rBV2	33849	57838	2.72%	0.363%
54	8.557	2252	2260	2261	rBV5	4643	5043	0.24%	0.032%
55	8.634	2272	2284	2306	rBV3	396629	952487	44.78%	5.985%
56	8.836	2340	2347	2359	rVB2	11800	20549	0.97%	0.129%
57	8.975	2387	2390	2393	rBV2	450	383	0.02%	0.002%
58	9.061	2414	2417	2420	rBV2	555	313	0.01%	0.002%
59	9.081	2420	2423	2429	rVB3	425	366	0.02%	0.002%
60	9.119	2431	2435	2439	rVB3	456	334	0.02%	0.002%
61	9.209	2451	2463	2479	rBV	85846	142631	6.70%	0.896%
62	9.367	2505	2512	2514	rBV2	1920	2052	0.10%	0.013%
63	9.415	2514	2527	2551	rVV	786499	1326424	62.35%	8.335%
64	9.608	2584	2587	2589	rBV2	438	299	0.01%	0.002%
65	9.647	2594	2599	2601	rBV6	842	588	0.03%	0.004%
66	9.695	2610	2614	2620	rBV3	881	947	0.04%	0.006%
67	9.852	2660	2663	2668	rBV3	358	340	0.02%	0.002%
68	9.930	2680	2687	2691	rBV	1340	1448	0.07%	0.009%
69	9.949	2691	2693	2698	rVV2	627	486	0.02%	0.003%
70	10.081	2724	2734	2738	rBV4	2990	4856	0.23%	0.031%
71	10.306	2799	2804	2807	rBV	389	282	0.01%	0.002%
72	10.505	2862	2866	2870	rVB2	377	372	0.02%	0.002%
73	10.637	2904	2907	2912	rVB2	445	375	0.02%	0.002%
74	10.753	2930	2943	2963	rBV	725593	1185662	55.74%	7.450%
75	10.868	2975	2979	2980	rBV2	637	362	0.02%	0.002%
76	10.926	2993	2997	3000	rBV2	498	394	0.02%	0.002%

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77	11.122	3056	3058	3065	rVB3	600	445	0.02%	0.003%
78	11.229	3086	3091	3095	rBV2	527	543	0.03%	0.003%
79	11.344	3120	3127	3132	rBV2	428	605	0.03%	0.004%
80	11.370	3132	3135	3140	rVB2	402	300	0.01%	0.002%
81	11.412	3146	3148	3155	rVB2	567	593	0.03%	0.004%
82	11.756	3251	3255	3258	rBV3	606	539	0.03%	0.003%
83	11.811	3259	3272	3299	rBV	763253	1237289	58.16%	7.774%
84	12.135	3369	3373	3375	rBV2	487	359	0.02%	0.002%
85	12.190	3375	3390	3412	rBV	905282	1485050	69.81%	9.331%
86	12.640	3527	3530	3535	rBV2	473	418	0.02%	0.003%
87	13.142	3683	3686	3690	rBV2	713	520	0.02%	0.003%
88	13.267	3722	3725	3728	rBV	498	398	0.02%	0.003%
89	13.302	3733	3736	3738	rBV2	583	333	0.02%	0.002%
90	13.376	3755	3759	3762	rBV2	401	321	0.02%	0.002%
91	13.470	3785	3788	3789	rBV	626	376	0.02%	0.002%
92	13.630	3837	3838	3845	rBV2	329	355	0.02%	0.002%
93	13.692	3855	3857	3860	rBV	467	292	0.01%	0.002%
94	13.724	3864	3867	3871	rBV2	678	535	0.03%	0.003%
95	13.836	3900	3902	3905	rBV	346	277	0.01%	0.002%
96	13.881	3914	3916	3919	rVB2	553	312	0.01%	0.002%
97	13.913	3923	3926	3931	rBV3	469	403	0.02%	0.003%
98	14.727	4177	4179	4185	rBV3	596	521	0.02%	0.003%
99	15.254	4341	4343	4348	rBV4	840	669	0.03%	0.004%
100	15.389	4382	4385	4386	rBV2	1155	523	0.02%	0.003%

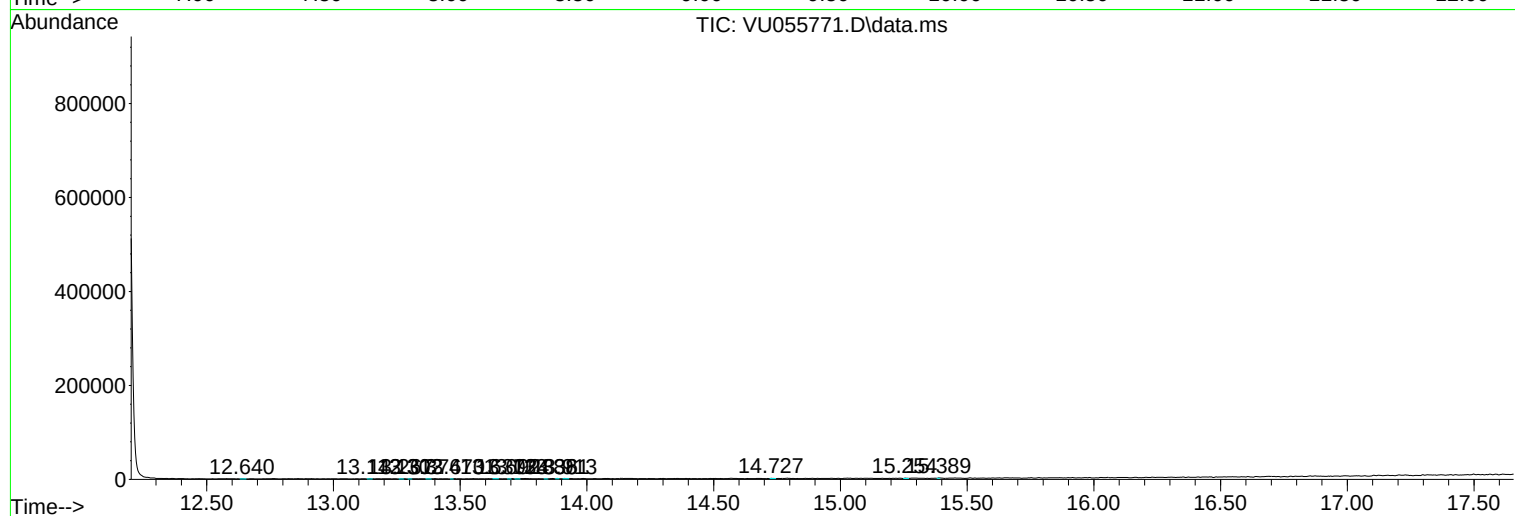
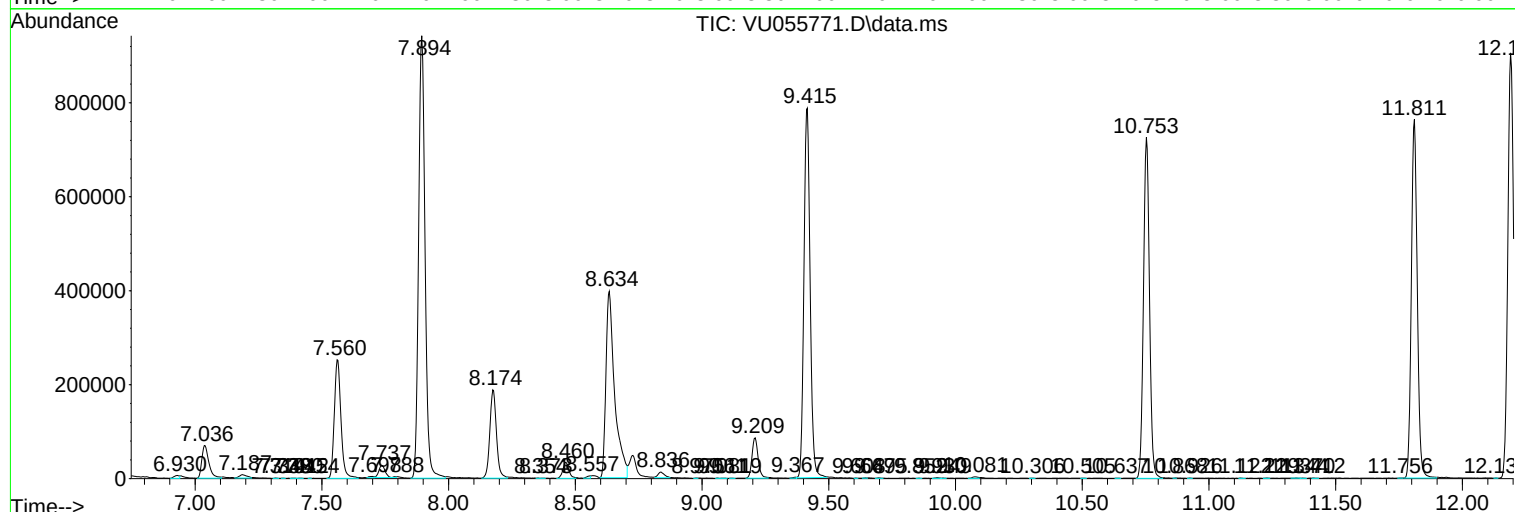
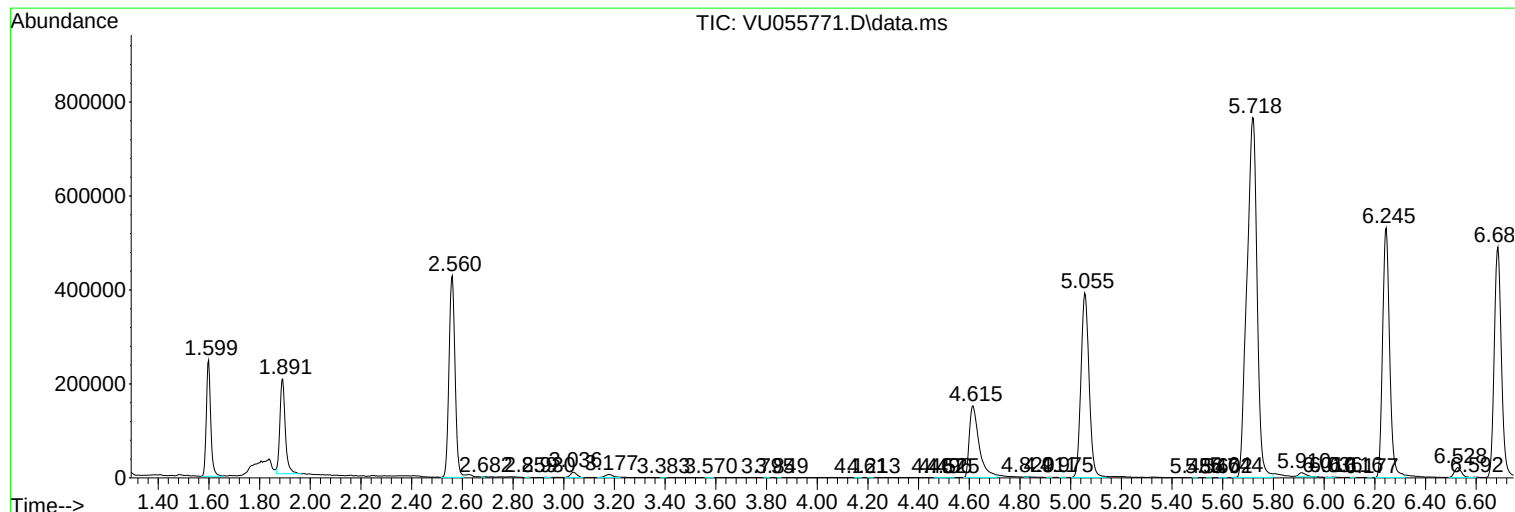
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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



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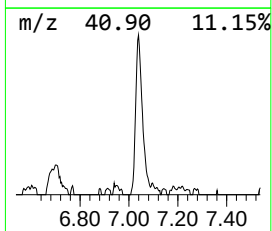
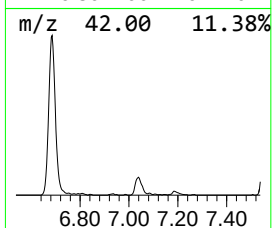
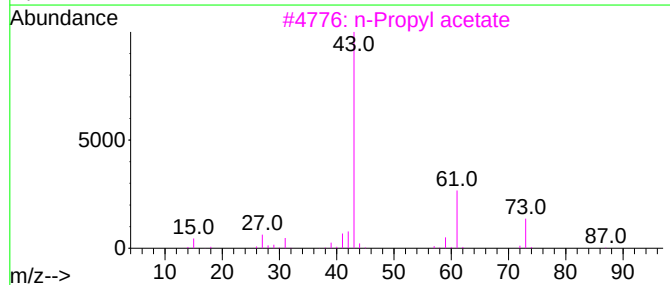
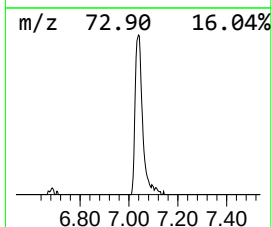
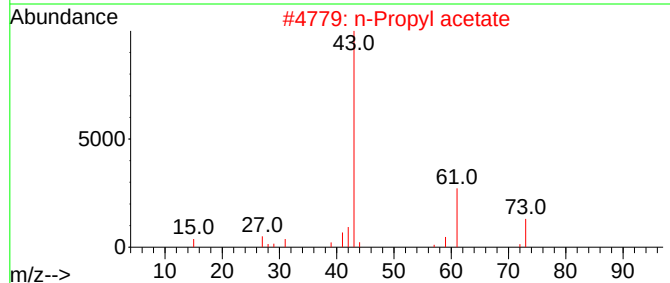
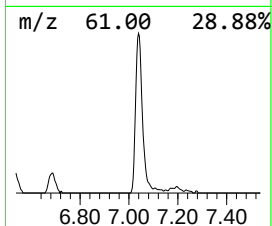
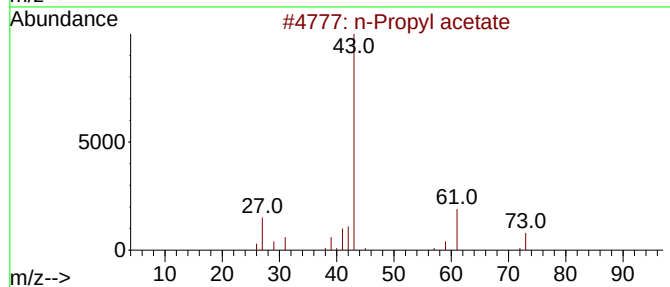
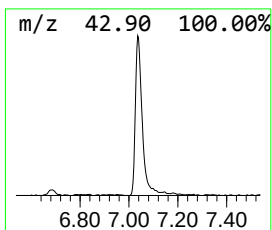
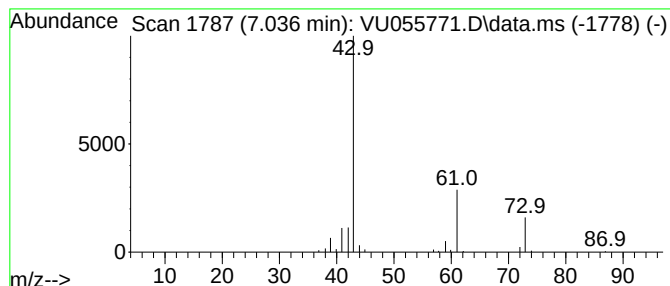
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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	6.49 ug/L	133747	1,4-Difluorobenzene	6.245

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	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	74
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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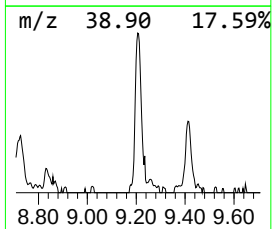
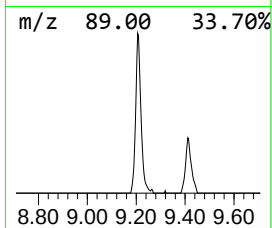
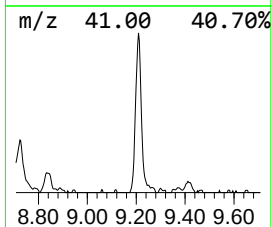
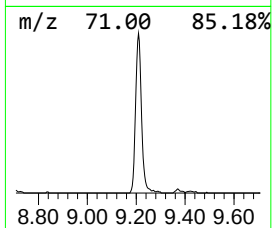
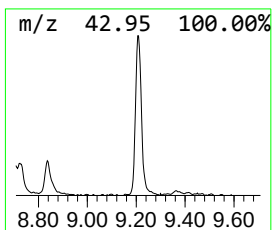
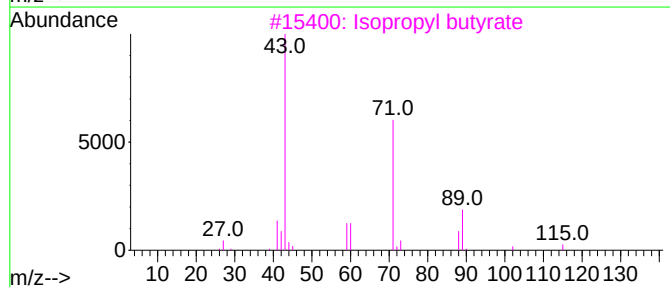
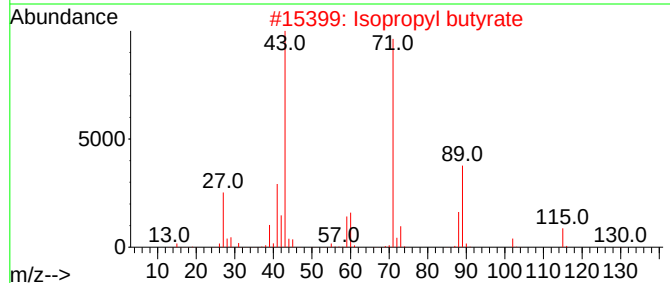
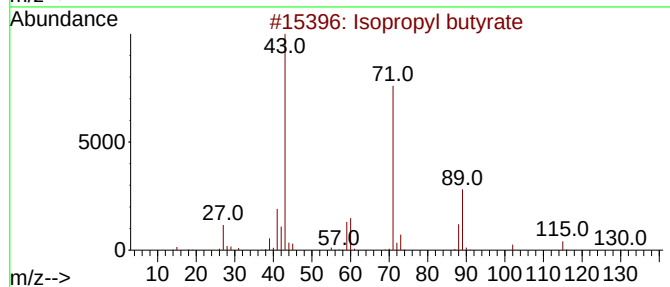
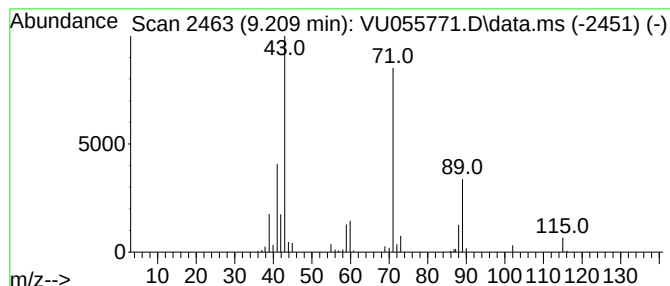
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Quant Title : VOC Analysis

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	5.38 ug/L	142631	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	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



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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	7.036	6.5	ug/L	133747	1	6.245	1030920	50.0
Isopropyl butyrate	9.209	5.4	ug/L	142631	2	9.415	1326420	50.0