

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
 Data File : VU049679.D
 Acq On : 11 Jul 2022 16:32
 Operator : SY/MD
 Sample : PB146107TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB107

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\SFAMULM071122WMA.M
 Title : VOC Analysis

Signal : TIC: VU049679.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	96	rBV	123713	135904	13.88%	1.820%
2	1.899	166	174	199	rVB	88270	123554	12.62%	1.655%
3	2.562	368	380	394	rBV	176215	283181	28.93%	3.793%
4	2.732	430	433	434	rBV	262	149	0.02%	0.002%
5	3.002	514	517	519	rBV2	181	102	0.01%	0.001%
6	3.041	519	529	540	rBV2	9210	16620	1.70%	0.223%
7	3.179	558	572	589	rBV2	11476	26550	2.71%	0.356%
8	3.539	681	684	687	rBV	203	145	0.01%	0.002%
9	3.639	710	715	719	rVB2	224	217	0.02%	0.003%
10	3.684	727	729	731	rBV2	117	66	0.01%	0.001%
11	3.755	748	751	752	rBV	136	83	0.01%	0.001%
12	3.880	786	790	794	rBV	233	206	0.02%	0.003%
13	3.932	802	806	810	rBV2	197	171	0.02%	0.002%
14	3.989	821	824	826	rBV	105	60	0.01%	0.001%
15	4.002	826	828	830	rVB	116	51	0.01%	0.001%
16	4.015	830	832	834	rBV	55	20	0.00%	0.000%
17	4.034	835	838	840	rBV	116	71	0.01%	0.001%
18	4.067	845	848	851	rBV	166	96	0.01%	0.001%
19	4.121	863	865	866	rBV	136	40	0.00%	0.001%
20	4.169	876	880	883	rBV2	245	263	0.03%	0.004%
21	4.192	883	887	891	rVB2	403	337	0.03%	0.005%
22	4.211	891	893	894	rBV	86	39	0.00%	0.001%
23	4.276	908	913	916	rBV	251	254	0.03%	0.003%
24	4.327	926	929	935	rBV2	178	190	0.02%	0.003%
25	4.414	953	956	959	rBV	172	146	0.01%	0.002%
26	4.468	970	973	977	rBV	153	103	0.01%	0.001%
27	4.485	977	978	979	rBV	116	29	0.00%	0.000%
28	4.546	995	997	999	rBV	184	126	0.01%	0.002%
29	4.620	1006	1020	1045	rBV	119683	289475	29.57%	3.877%
30	5.060	1141	1157	1177	rBV	177608	385354	39.37%	5.161%
31	5.179	1191	1194	1195	rBV2	215	113	0.01%	0.002%
32	5.224	1204	1208	1210	rBV2	302	180	0.02%	0.002%
33	5.266	1217	1221	1222	rBV2	242	171	0.02%	0.002%
34	5.285	1222	1227	1231	rVV2	608	817	0.08%	0.011%
35	5.330	1238	1241	1244	rBV2	97	64	0.01%	0.001%
36	5.366	1249	1252	1263	rVB4	589	1019	0.10%	0.014%

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 Title : VOC Analysis

37	5.414	1263	1267	1268	rBV2	141	94	0.01%	0.001%
38	5.427	1268	1271	1273	rBV	140	92	0.01%	0.001%
39	5.475	1282	1286	1289	rBV	337	209	0.02%	0.003%
40	5.523	1298	1301	1303	rBV	236	134	0.01%	0.002%
41	5.552	1307	1310	1312	rBV	165	94	0.01%	0.001%
42	5.568	1312	1315	1318	rBV	254	153	0.02%	0.002%
43	5.722	1341	1363	1382	rBV2	360934	978788	100.00%	13.110%
44	5.912	1414	1422	1434	rVB2	4356	7735	0.79%	0.104%
45	6.108	1481	1483	1484	rBB	32	23	0.00%	0.000%
46	6.118	1484	1486	1488	rVB2	185	84	0.01%	0.001%
47	6.153	1493	1497	1502	rBV3	200	229	0.02%	0.003%
48	6.247	1511	1526	1550	rBV	299091	557341	56.94%	7.465%
49	6.411	1575	1577	1580	rBV	240	124	0.01%	0.002%
50	6.526	1610	1613	1618	rBV3	798	756	0.08%	0.010%
51	6.578	1626	1629	1630	rBV	225	82	0.01%	0.001%
52	6.597	1630	1635	1639	rVB3	421	381	0.04%	0.005%
53	6.690	1649	1664	1682	rBV	236341	457390	46.73%	6.126%
54	6.925	1728	1737	1751	rBV2	3541	7168	0.73%	0.096%
55	6.989	1756	1757	1758	rBV2	124	33	0.00%	0.000%
56	7.038	1761	1772	1791	rBV	51309	90797	9.28%	1.216%
57	7.218	1825	1828	1833	rVB2	431	301	0.03%	0.004%
58	7.247	1833	1837	1842	rVB2	343	270	0.03%	0.004%
59	7.272	1842	1845	1847	rVB2	284	160	0.02%	0.002%
60	7.288	1847	1850	1852	rBV	93	41	0.00%	0.001%
61	7.314	1855	1858	1859	rBV	201	85	0.01%	0.001%
62	7.337	1863	1865	1868	rBV	87	44	0.00%	0.001%
63	7.353	1868	1870	1872	rBV	184	85	0.01%	0.001%
64	7.423	1890	1892	1894	rBV2	63	33	0.00%	0.000%
65	7.449	1898	1900	1905	rVB2	124	86	0.01%	0.001%
66	7.475	1905	1908	1910	rBV2	96	69	0.01%	0.001%
67	7.565	1923	1936	1957	rBV	116446	206441	21.09%	2.765%
68	7.684	1971	1973	1975	rBV	268	189	0.02%	0.003%
69	7.738	1978	1990	2001	rBV2	9814	15974	1.63%	0.214%
70	7.896	2026	2039	2056	rBV	410922	710287	72.57%	9.514%
71	8.121	2104	2109	2110	rBV	210	195	0.02%	0.003%
72	8.179	2111	2127	2145	rVV2	82979	153043	15.64%	2.050%
73	8.394	2191	2194	2199	rVB2	217	148	0.02%	0.002%
74	8.465	2206	2216	2228	rBV2	12402	20432	2.09%	0.274%
75	8.526	2232	2235	2237	rBV	305	206	0.02%	0.003%
76	8.552	2237	2243	2246	rBV4	2848	3247	0.33%	0.043%

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77	8.632	2257	2268	2290	rBV2	332384	589212	60.20%	7.892%
78	8.835	2323	2331	2344	rVB2	13672	21164	2.16%	0.283%
79	8.951	2365	2367	2370	rBV2	246	104	0.01%	0.001%
80	9.127	2417	2422	2426	rBV2	231	249	0.03%	0.003%
81	9.211	2438	2448	2458	rBV	37988	58798	6.01%	0.788%
82	9.369	2491	2497	2500	rBV4	1102	1314	0.13%	0.018%
83	9.417	2500	2512	2543	rVB	406712	667982	68.25%	8.947%
84	9.925	2663	2670	2678	rVB4	1149	1608	0.16%	0.022%
85	10.005	2692	2695	2697	rBV	205	129	0.01%	0.002%
86	10.073	2709	2716	2724	rBV4	2004	3073	0.31%	0.041%
87	10.137	2731	2736	2740	rBV3	387	433	0.04%	0.006%
88	10.561	2864	2868	2870	rBV	310	281	0.03%	0.004%
89	10.754	2916	2928	2947	rBV	307176	494291	50.50%	6.621%
90	11.047	3017	3019	3021	rBV	230	82	0.01%	0.001%
91	11.812	3244	3257	3279	rBV	355949	570504	58.29%	7.641%
92	12.024	3320	3323	3330	rBV2	327	471	0.05%	0.006%
93	12.127	3351	3355	3358	rBV2	469	445	0.05%	0.006%
94	12.192	3363	3375	3399	rVV	354159	576882	58.94%	7.727%

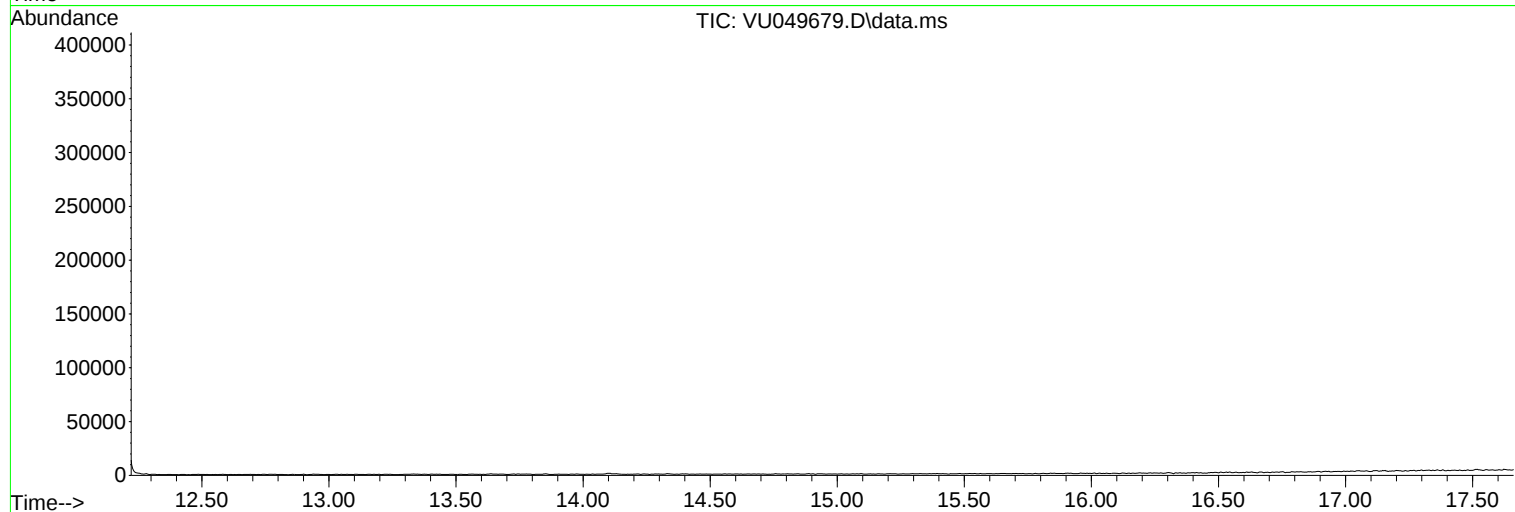
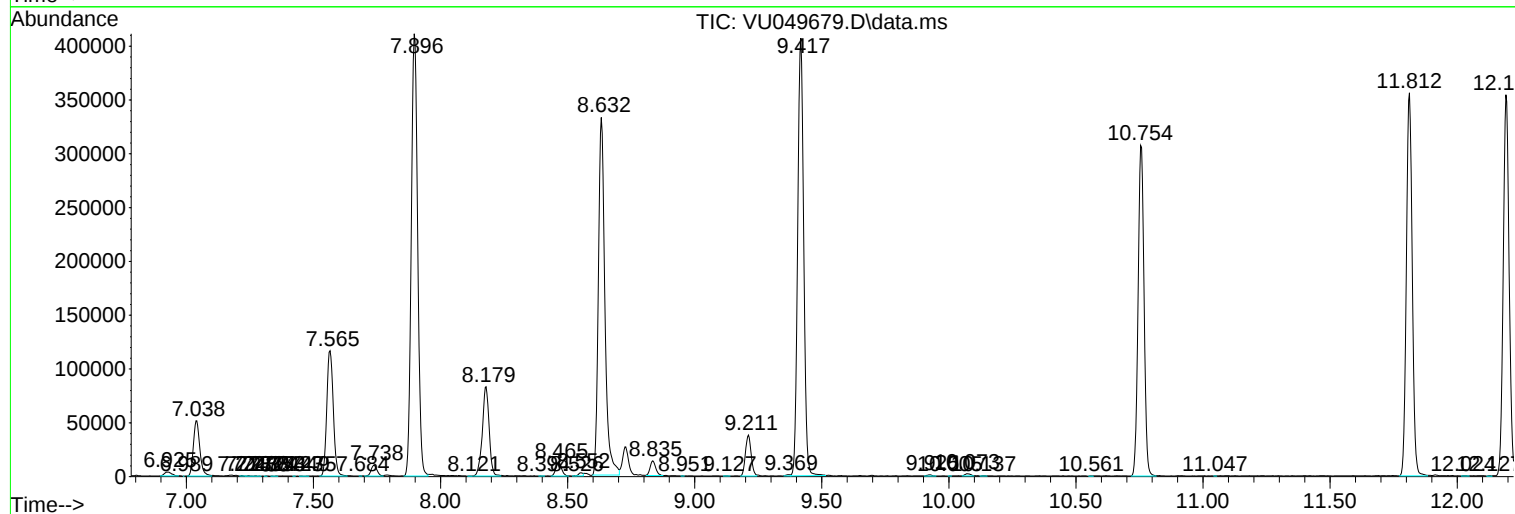
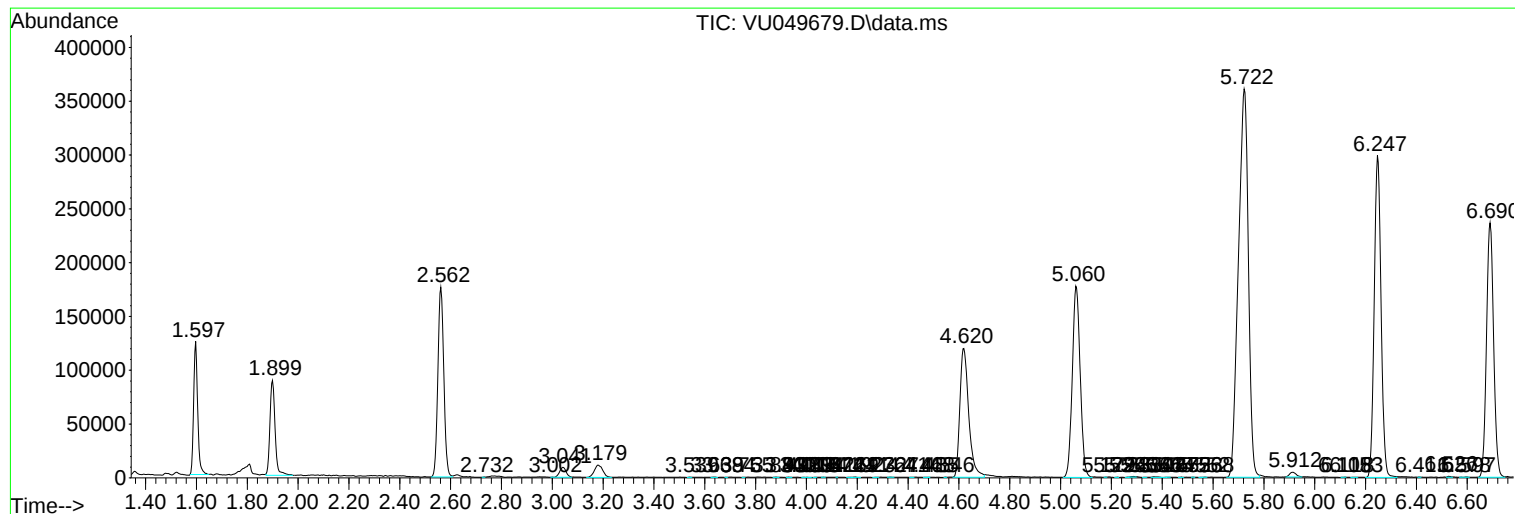
Sum of corrected areas: 7466031

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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



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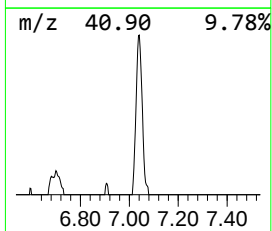
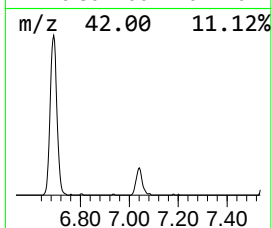
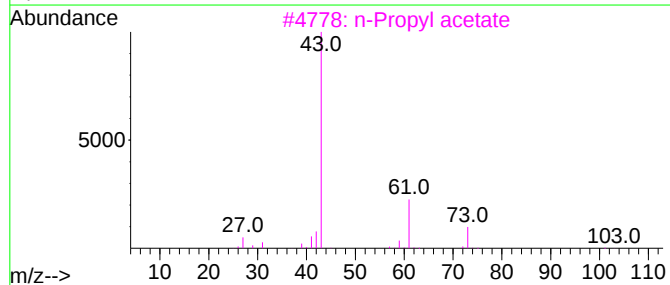
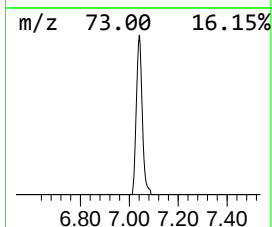
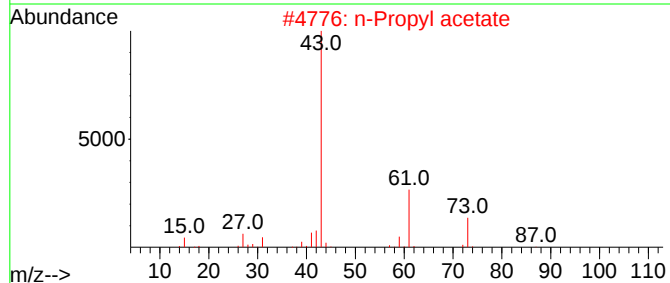
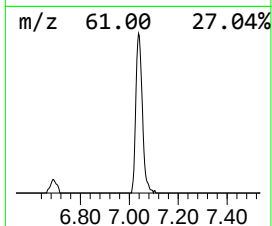
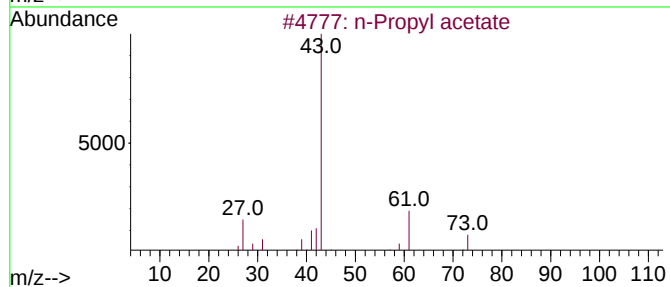
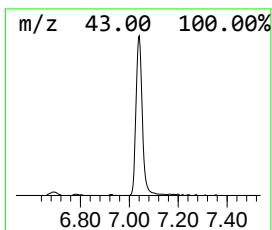
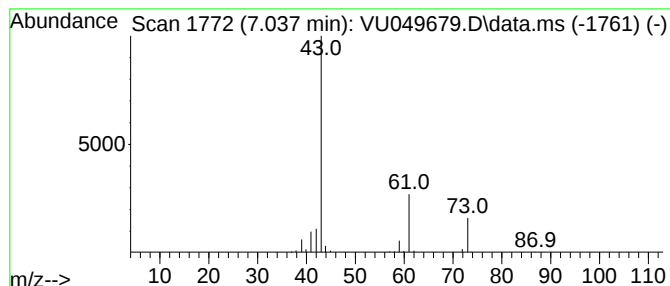
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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.
7.037	8.15 ug/L	90797	1,4-Difluorobenzene	6.247

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



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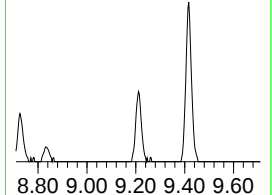
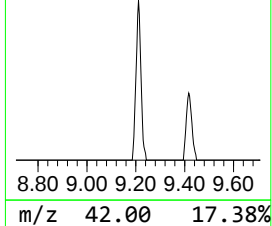
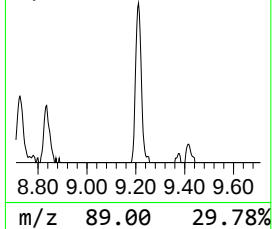
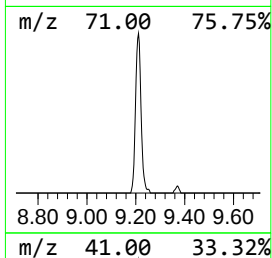
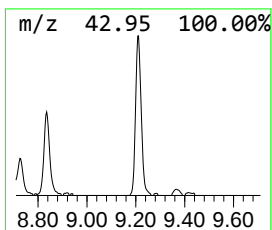
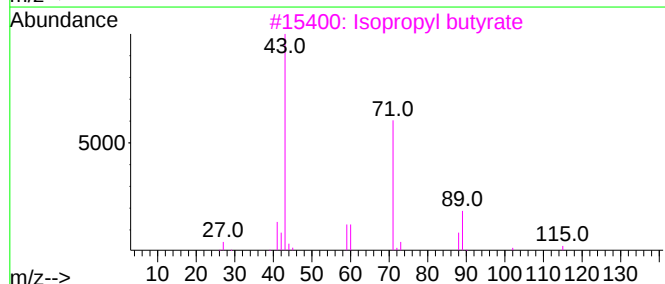
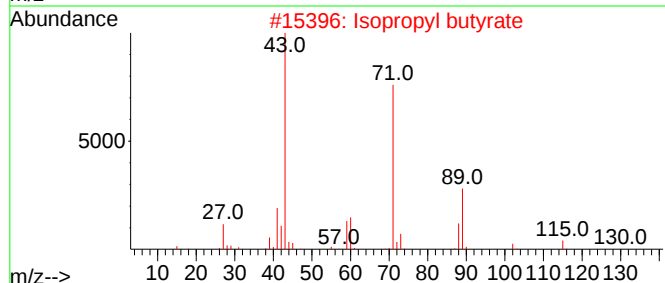
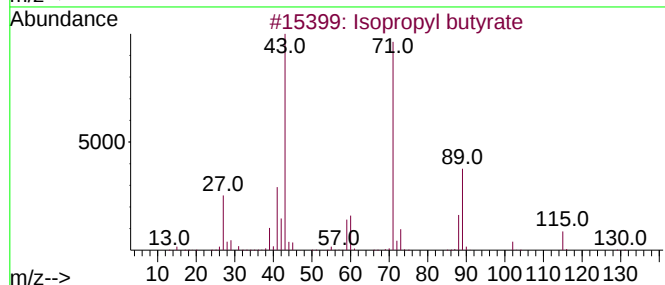
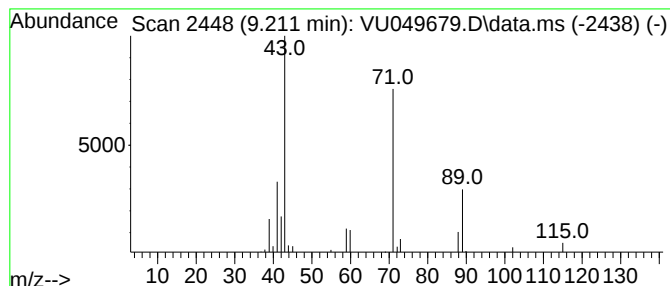
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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.
9.211	4.40 ug/L	58798	Chlorobenzene-d5	9.417

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	83
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.037	8.2	ug/L	90797	1	6.247	557341	50.0
Isopropyl butyrate	9.211	4.4	ug/L	58798	2	9.417	667982	50.0