

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
 Data File : VU055775.D
 Acq On : 16 Oct 2023 16:25
 Operator : MD/SY
 Sample : 04874-03 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COM27

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: VU055775.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	111	rBV	199408	241415	12.84%	1.643%
2	1.888	178	186	205	rVB	166819	247724	13.18%	1.686%
3	2.557	378	394	409	rBV	345334	570143	30.33%	3.880%
4	2.702	435	439	441	rBV3	810	667	0.04%	0.005%
5	2.933	505	511	513	rVV3	422	428	0.02%	0.003%
6	2.985	525	527	532	rVB2	712	450	0.02%	0.003%
7	3.036	532	543	555	rBV2	13611	25132	1.34%	0.171%
8	3.177	571	587	601	rBV	15998	38087	2.03%	0.259%
9	3.268	613	615	621	rVB3	568	381	0.02%	0.003%
10	3.499	685	687	693	rVV2	397	330	0.02%	0.002%
11	3.579	709	712	716	rVB	474	349	0.02%	0.002%
12	3.663	735	738	742	rBV2	376	286	0.02%	0.002%
13	3.702	747	750	757	rVV3	444	419	0.02%	0.003%
14	3.975	832	835	839	rVB2	675	473	0.03%	0.003%
15	4.013	844	847	850	rVV2	419	323	0.02%	0.002%
16	4.030	850	852	857	rVV2	415	357	0.02%	0.002%
17	4.357	951	954	960	rBV2	296	323	0.02%	0.002%
18	4.557	1012	1016	1019	rBV	441	368	0.02%	0.003%
19	4.615	1019	1034	1065	rBV	127914	351448	18.70%	2.392%
20	5.055	1154	1171	1196	rBV	317491	711343	37.85%	4.841%
21	5.325	1248	1255	1256	rBV5	1030	1111	0.06%	0.008%
22	5.718	1354	1377	1411	rBV2	677392	1879542	100.00%	12.792%
23	5.910	1429	1437	1449	rBV3	7633	14697	0.78%	0.100%
24	6.039	1471	1477	1479	rBV4	868	666	0.04%	0.005%
25	6.242	1525	1540	1570	rBV	574832	1123441	59.77%	7.646%
26	6.396	1586	1588	1591	rVB2	944	448	0.02%	0.003%
27	6.425	1595	1597	1600	rVB2	816	371	0.02%	0.003%
28	6.460	1605	1608	1610	rBV2	616	368	0.02%	0.003%
29	6.528	1618	1629	1644	rBV3	18918	36246	1.93%	0.247%
30	6.592	1646	1649	1652	rBV4	713	540	0.03%	0.004%
31	6.685	1663	1678	1701	rBV	430434	853064	45.39%	5.806%
32	6.933	1745	1755	1766	rBV	6451	14947	0.80%	0.102%
33	7.039	1778	1788	1812	rBV	46473	92072	4.90%	0.627%
34	7.190	1822	1835	1843	rBV6	6379	13674	0.73%	0.093%
35	7.296	1863	1868	1870	rBV2	526	489	0.03%	0.003%
36	7.383	1891	1895	1899	rBV2	593	429	0.02%	0.003%

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 Title : VOC Analysis

37	7.418	1902	1906	1908	rBV2	475	331	0.02%	0.002%
38	7.486	1924	1927	1929	rBV	420	306	0.02%	0.002%
39	7.560	1938	1950	1979	rBV	224894	405714	21.59%	2.761%
40	7.698	1985	1993	1996	rBV4	3241	4899	0.26%	0.033%
41	7.737	1997	2005	2017	rVB2	23222	40486	2.15%	0.276%
42	7.894	2039	2054	2086	rBV	812733	1448072	77.04%	9.855%
43	8.039	2097	2099	2104	rVB3	1092	493	0.03%	0.003%
44	8.174	2125	2141	2167	rBV	167520	297313	15.82%	2.023%
45	8.306	2180	2182	2188	rVB3	872	690	0.04%	0.005%
46	8.335	2188	2191	2195	rBV3	562	482	0.03%	0.003%
47	8.386	2204	2207	2210	rVB2	500	313	0.02%	0.002%
48	8.463	2220	2231	2244	rVV3	29232	50407	2.68%	0.343%
49	8.563	2252	2262	2263	rBV6	4970	5883	0.31%	0.040%
50	8.634	2272	2284	2307	rBV3	364674	861347	45.83%	5.862%
51	8.836	2340	2347	2358	rBV3	5126	8760	0.47%	0.060%
52	8.920	2371	2373	2376	rVB3	744	306	0.02%	0.002%
53	9.209	2452	2463	2480	rBV	65675	111622	5.94%	0.760%
54	9.364	2505	2511	2513	rVV	1257	1205	0.06%	0.008%
55	9.415	2514	2527	2563	rVB	862798	1457284	77.53%	9.918%
56	9.569	2571	2575	2580	rVB3	804	822	0.04%	0.006%
57	9.615	2586	2589	2594	rVB3	759	610	0.03%	0.004%
58	9.640	2594	2597	2599	rVB2	574	308	0.02%	0.002%
59	9.650	2599	2600	2607	rVB2	571	461	0.02%	0.003%
60	9.692	2607	2613	2615	rBV2	987	881	0.05%	0.006%
61	9.766	2634	2636	2640	rVB3	390	295	0.02%	0.002%
62	9.795	2640	2645	2647	rBV2	469	339	0.02%	0.002%
63	9.830	2652	2656	2662	rBV	590	624	0.03%	0.004%
64	9.859	2662	2665	2668	rBV	565	386	0.02%	0.003%
65	9.930	2680	2687	2691	rBV2	1198	1420	0.08%	0.010%
66	9.971	2698	2700	2706	rVB2	374	306	0.02%	0.002%
67	10.055	2719	2726	2728	rBV	397	427	0.02%	0.003%
68	10.078	2728	2733	2736	rBV4	1436	1596	0.08%	0.011%
69	10.418	2837	2839	2843	rVB2	481	319	0.02%	0.002%
70	10.479	2855	2858	2861	rBV2	553	350	0.02%	0.002%
71	10.753	2926	2943	2964	rBV	654376	1068824	56.87%	7.274%
72	11.004	3018	3021	3028	rVB2	552	447	0.02%	0.003%
73	11.036	3028	3031	3035	rBV2	379	301	0.02%	0.002%
74	11.061	3035	3039	3044	rBV	360	346	0.02%	0.002%
75	11.168	3070	3072	3075	rVV	481	284	0.02%	0.002%
76	11.196	3078	3081	3085	rVB2	488	394	0.02%	0.003%

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77	11.248	3093	3097	3101	rVB2	347	337	0.02%	0.002%
78	11.412	3142	3148	3152	rVB3	1071	981	0.05%	0.007%
79	11.438	3152	3156	3159	rBV	445	426	0.02%	0.003%
80	11.528	3181	3184	3188	rBV	352	346	0.02%	0.002%
81	11.618	3210	3212	3217	rVB2	408	341	0.02%	0.002%
82	11.701	3234	3238	3242	rBV2	410	409	0.02%	0.003%
83	11.746	3250	3252	3256	rVB2	617	403	0.02%	0.003%
84	11.811	3259	3272	3302	rBV	846636	1360874	72.40%	9.262%
85	12.061	3348	3350	3355	rVB	595	414	0.02%	0.003%
86	12.103	3360	3363	3364	rBV3	496	320	0.02%	0.002%
87	12.190	3377	3390	3414	rVV	795507	1324013	70.44%	9.011%
88	12.489	3479	3483	3486	rBV	593	447	0.02%	0.003%
89	12.923	3614	3618	3621	rBV3	593	590	0.03%	0.004%
90	12.939	3621	3623	3626	rBV3	358	282	0.02%	0.002%
91	12.981	3633	3636	3641	rBV3	285	306	0.02%	0.002%
92	13.016	3644	3647	3651	rVV3	403	332	0.02%	0.002%
93	13.174	3692	3696	3698	rBV3	661	560	0.03%	0.004%
94	13.251	3715	3720	3721	rBV	684	457	0.02%	0.003%
95	13.409	3766	3769	3773	rVB	878	514	0.03%	0.003%
96	13.499	3794	3797	3799	rBV	1088	746	0.04%	0.005%
97	14.122	3988	3991	3993	rBV3	537	313	0.02%	0.002%
98	14.521	4113	4115	4119	rVB3	779	421	0.02%	0.003%
99	14.714	4172	4175	4177	rBV2	888	594	0.03%	0.004%
100	15.158	4311	4313	4316	rBV2	811	554	0.03%	0.004%

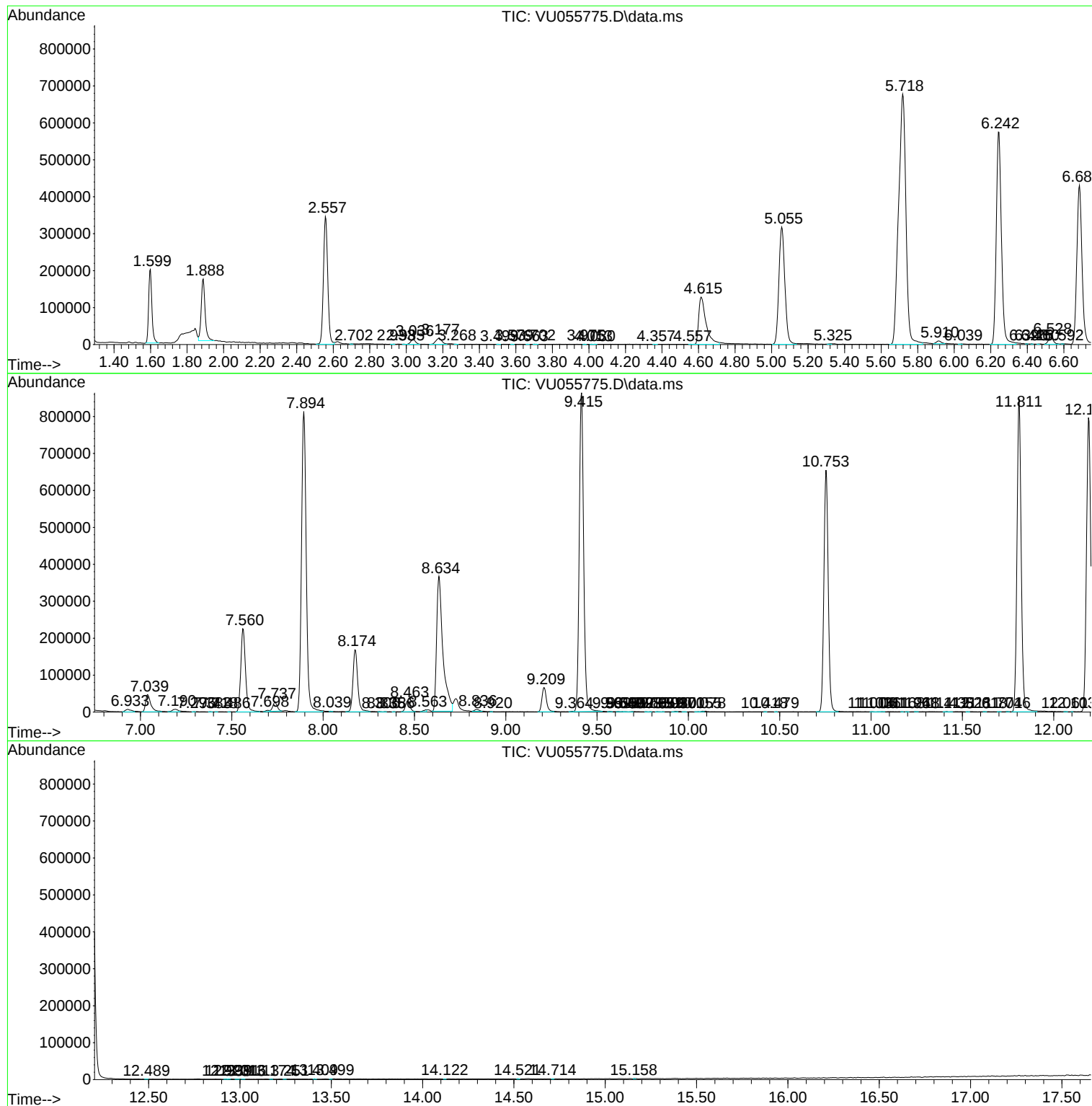
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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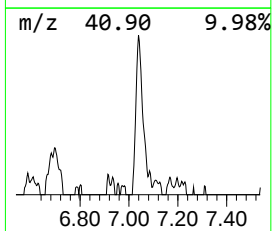
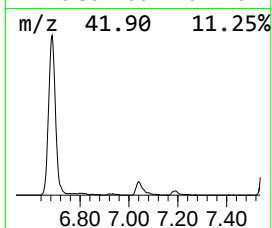
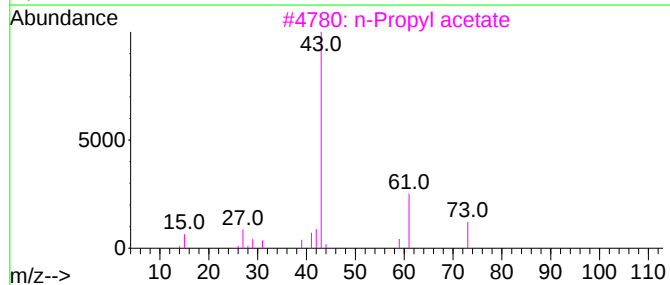
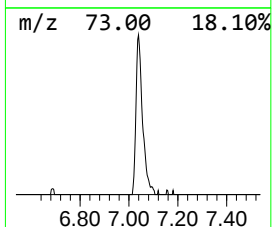
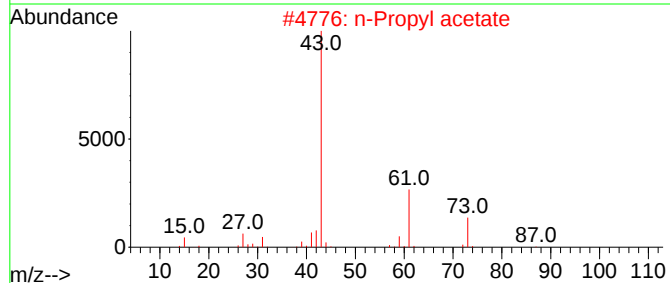
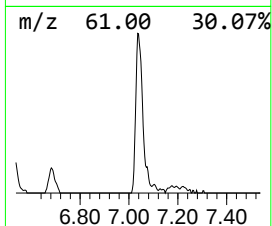
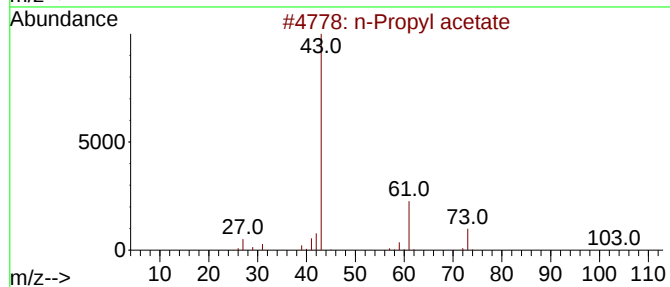
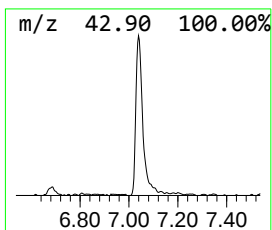
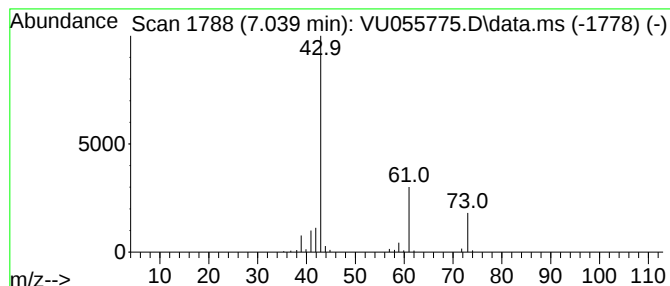
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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.
7.039	4.10 ug/L	92072	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	64
4	n-Propyl acetate			102	C5H10O2	000109-60-4	56
5	n-Propyl acetate			102	C5H10O2	000109-60-4	40



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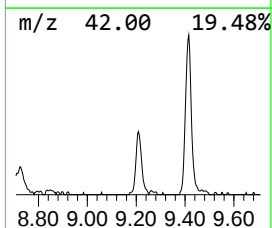
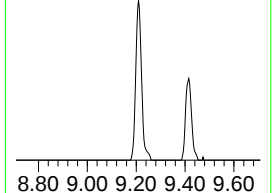
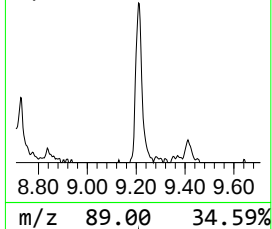
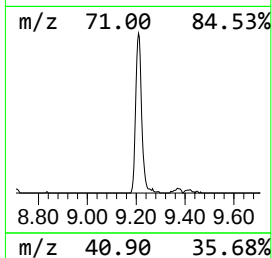
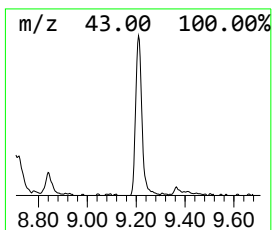
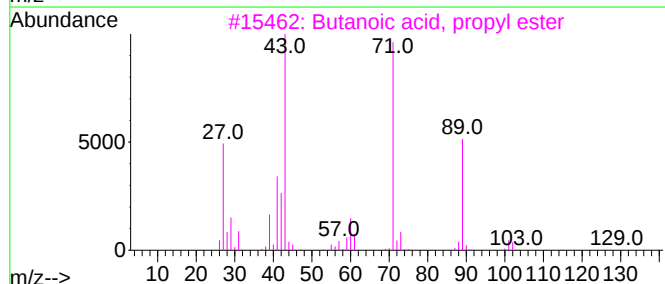
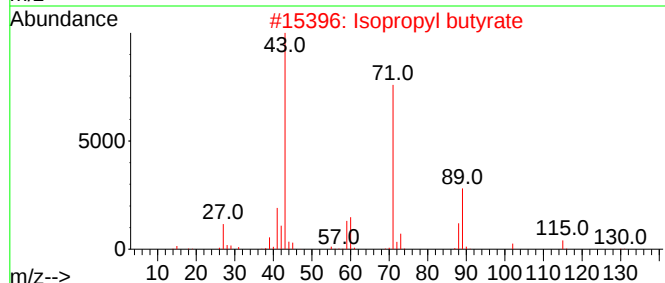
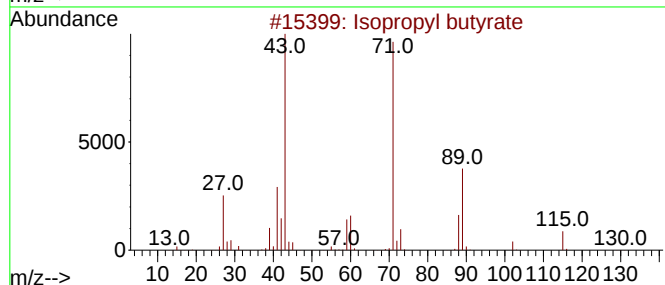
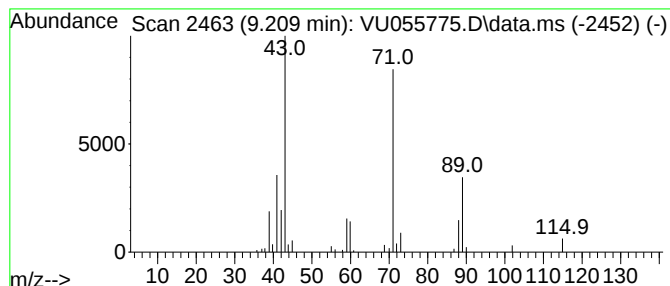
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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	3.83 ug/L	111622	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			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
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	7.039	4.1	ug/L	92072	1	6.245	1123440	50.0
Isopropyl butyrate	9.209	3.8	ug/L	111622	2	9.415	1457280	50.0