

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032724\
 Data File : VV034870.D
 Acq On : 27 Mar 2024 17:17
 Operator : SY/MD
 Sample : PB159796TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 19 Sample Multiplier: 1

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\SFAMVLM032624WMA.M

Title : VOC Analysis

Signal : TIC: VV034870.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	68	74	91	rVB	151250	159434	13.09%	1.574%
2	1.529	145	152	165	rVB	148611	174343	14.31%	1.721%
3	2.060	307	317	329	rBV	266798	391164	32.12%	3.861%
4	2.449	430	438	448	rVB3	6489	10228	0.84%	0.101%
5	2.539	464	466	470	rBV2	349	232	0.02%	0.002%
6	2.558	470	472	478	rVV3	443	414	0.03%	0.004%
7	2.619	487	491	493	rBV2	462	269	0.02%	0.003%
8	2.674	506	508	510	rBV2	425	173	0.01%	0.002%
9	2.767	535	537	540	rBV2	226	144	0.01%	0.001%
10	2.799	544	547	551	rBV4	254	223	0.02%	0.002%
11	2.941	586	591	595	rBV2	257	291	0.02%	0.003%
12	3.011	609	613	615	rBV	272	155	0.01%	0.002%
13	3.031	617	619	624	rVB4	299	217	0.02%	0.002%
14	3.063	624	629	630	rBV2	329	212	0.02%	0.002%
15	3.330	710	712	720	rVB	441	363	0.03%	0.004%
16	3.384	725	729	731	rBV2	422	303	0.02%	0.003%
17	3.410	731	737	740	rBV4	340	447	0.04%	0.004%
18	3.471	752	756	759	rVB	415	198	0.02%	0.002%
19	3.484	759	760	763	rVB	337	132	0.01%	0.001%
20	3.503	763	766	767	rBV	426	185	0.02%	0.002%
21	3.593	790	794	797	rBV2	302	222	0.02%	0.002%
22	3.680	819	821	823	rBV2	360	207	0.02%	0.002%
23	3.719	829	833	835	rBV2	257	206	0.02%	0.002%
24	3.783	845	853	889	rBV	99251	277506	22.78%	2.739%
25	4.246	982	997	1032	rBV	198791	515332	42.31%	5.087%
26	4.542	1087	1089	1092	rBV2	469	288	0.02%	0.003%
27	4.677	1129	1131	1133	rBV	344	205	0.02%	0.002%
28	4.822	1173	1176	1177	rBV	437	188	0.02%	0.002%
29	4.896	1196	1199	1200	rBV	272	148	0.01%	0.001%
30	4.957	1202	1218	1253	rBV2	452014	1217954	100.00%	12.023%
31	5.217	1293	1299	1311	rBV5	4624	9973	0.82%	0.098%
32	5.429	1363	1365	1371	rVB4	727	687	0.06%	0.007%
33	5.532	1386	1397	1428	rBV	374261	781639	64.18%	7.716%
34	5.831	1480	1490	1509	rBV3	9610	22351	1.84%	0.221%
35	5.921	1516	1518	1523	rBV3	495	375	0.03%	0.004%
36	5.989	1525	1539	1567	rBV	275207	578420	47.49%	5.710%

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 Title : VOC Analysis

37	6.269	1624	1626	1629	rBV4	513	256	0.02%	0.003%
38	6.394	1658	1665	1701	rBV	69950	149219	12.25%	1.473%
39	6.912	1815	1826	1852	rBV	142679	276090	22.67%	2.725%
40	7.124	1883	1892	1910	rBV	18663	35416	2.91%	0.350%
41	7.243	1918	1929	1954	rBV	500672	892054	73.24%	8.806%
42	7.551	2016	2025	2052	rBV	118929	225813	18.54%	2.229%
43	7.863	2108	2122	2138	rBV2	24738	46374	3.81%	0.458%
44	7.976	2150	2157	2162	rBV4	5743	8073	0.66%	0.080%
45	8.024	2163	2172	2199	rVV	323090	627681	51.54%	6.196%
46	8.249	2236	2242	2256	rBV2	17250	28762	2.36%	0.284%
47	8.545	2333	2334	2336	rBV2	506	225	0.02%	0.002%
48	8.619	2347	2357	2378	rBV	72207	123326	10.13%	1.217%
49	8.783	2398	2408	2440	rBV	605777	994410	81.65%	9.816%
50	9.172	2526	2529	2530	rBV2	556	276	0.02%	0.003%
51	9.349	2582	2584	2590	rBV4	630	588	0.05%	0.006%
52	9.455	2615	2617	2619	rBV3	492	237	0.02%	0.002%
53	9.497	2624	2630	2632	rBV4	3311	3384	0.28%	0.033%
54	9.654	2676	2679	2680	rVB2	385	173	0.01%	0.002%
55	9.696	2690	2692	2693	rBV	420	212	0.02%	0.002%
56	9.966	2774	2776	2780	rBV2	422	259	0.02%	0.003%
57	9.985	2780	2782	2785	rBV	478	318	0.03%	0.003%
58	10.072	2805	2809	2811	rBV2	404	293	0.02%	0.003%
59	10.153	2821	2834	2860	rBV	433840	697057	57.23%	6.881%
60	10.333	2888	2890	2894	rVB2	491	286	0.02%	0.003%
61	10.481	2933	2936	2943	rBV3	622	525	0.04%	0.005%
62	10.513	2943	2946	2948	rVB2	387	170	0.01%	0.002%
63	10.545	2953	2956	2960	rVB	566	355	0.03%	0.004%
64	10.641	2985	2986	2989	rVB2	325	143	0.01%	0.001%
65	10.661	2991	2992	2996	rVB3	401	175	0.01%	0.002%
66	10.838	3045	3047	3050	rBV2	301	154	0.01%	0.002%
67	10.857	3051	3053	3058	rBV4	578	517	0.04%	0.005%
68	10.956	3080	3084	3087	rBV2	353	345	0.03%	0.003%
69	11.059	3112	3116	3119	rBV2	435	324	0.03%	0.003%
70	11.185	3144	3155	3184	rBV	607193	944954	77.59%	9.328%
71	11.493	3249	3251	3253	rBV3	437	257	0.02%	0.003%
72	11.558	3259	3271	3297	rBV	584089	919788	75.52%	9.079%
73	11.712	3317	3319	3321	rBV3	673	404	0.03%	0.004%
74	11.873	3367	3369	3370	rVB	435	123	0.01%	0.001%
75	11.889	3370	3374	3375	rBV2	342	211	0.02%	0.002%
76	11.928	3383	3386	3388	rBV	493	221	0.02%	0.002%

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 Title : VOC Analysis

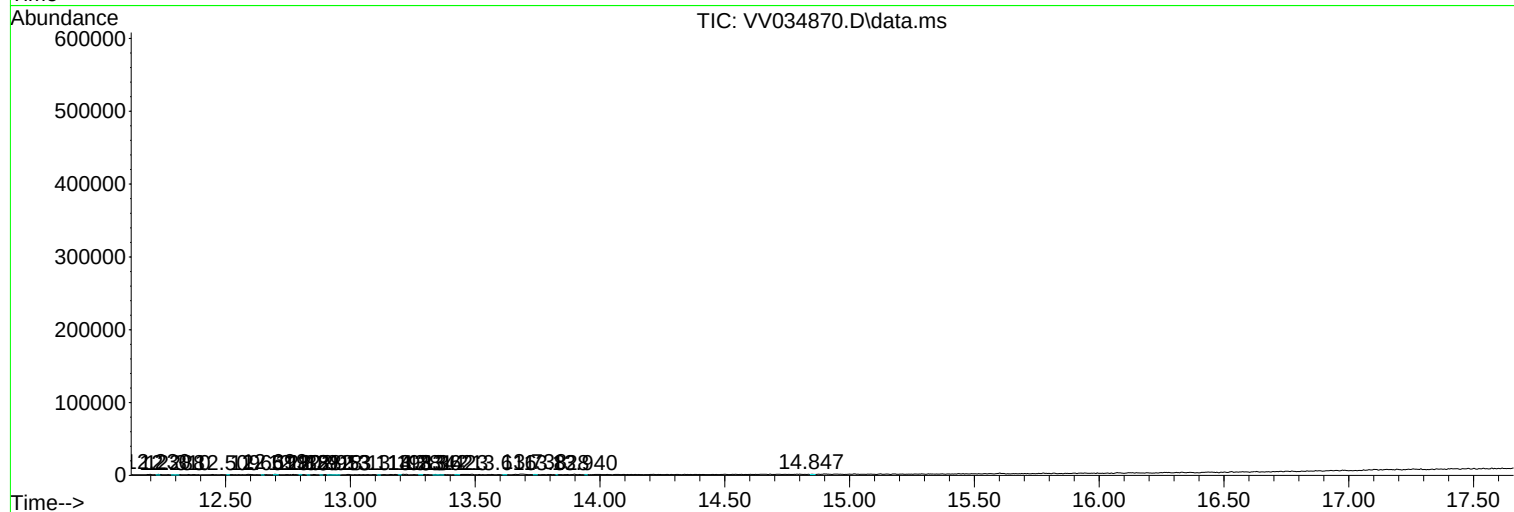
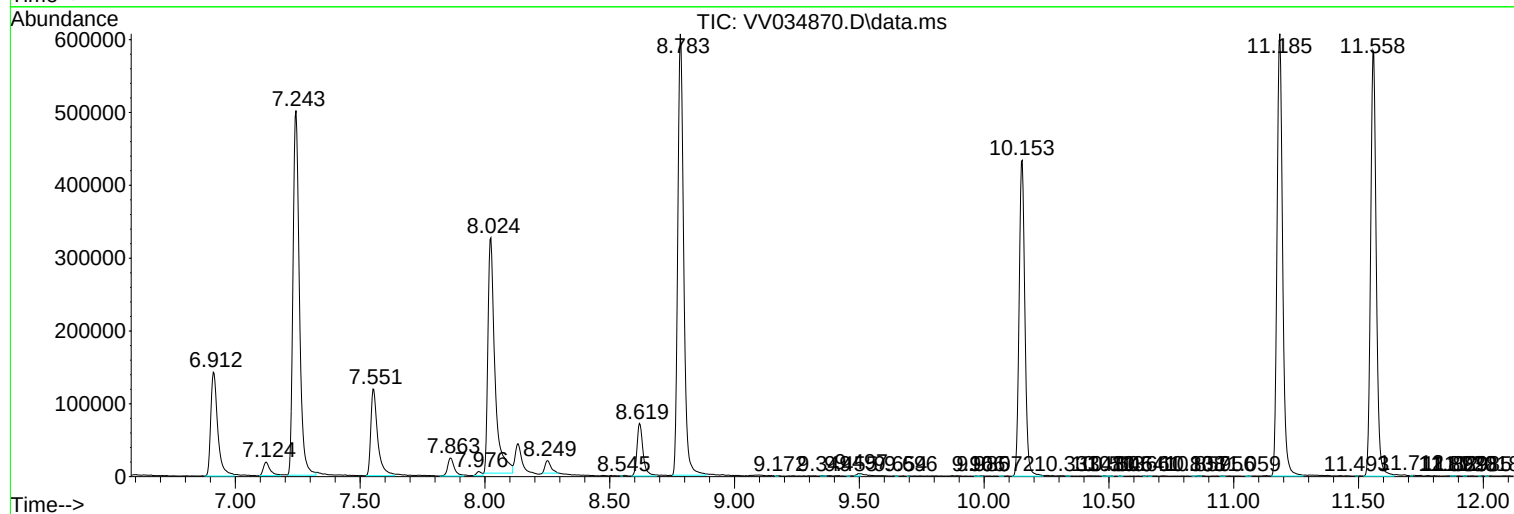
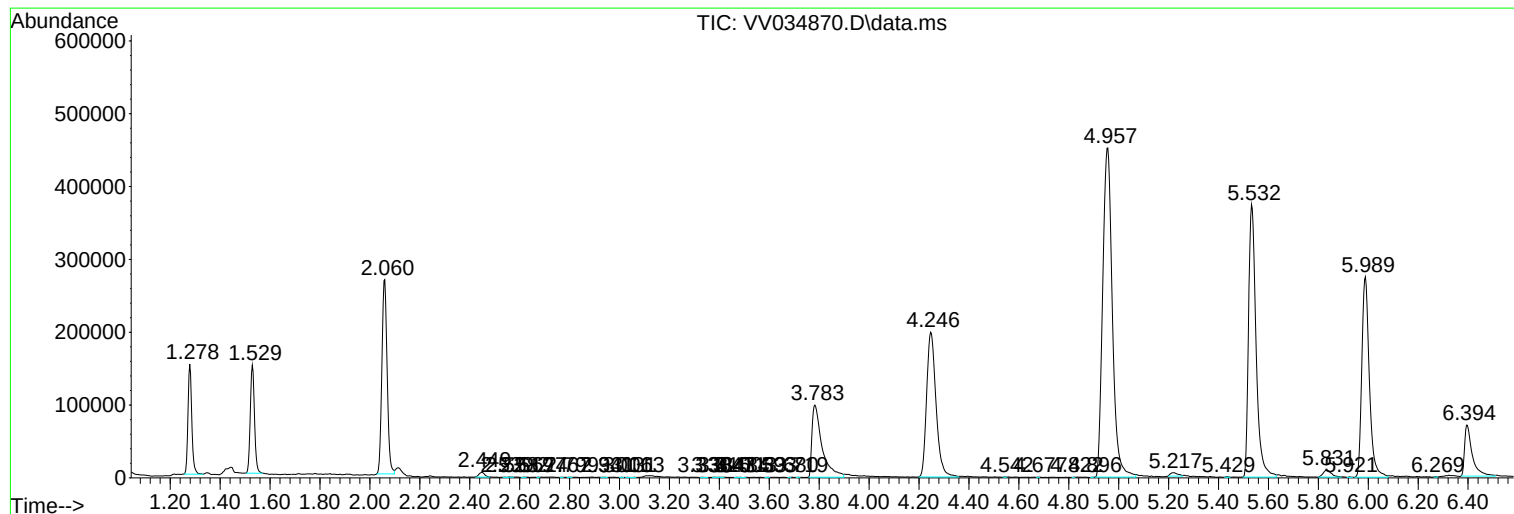
77	11.985	3402	3404	3406	rBV2	377	212	0.02%	0.002%
78	12.018	3411	3414	3415	rBV2	341	193	0.02%	0.002%
79	12.230	3477	3480	3482	rBV2	695	389	0.03%	0.004%
80	12.288	3496	3498	3501	rVB2	341	149	0.01%	0.001%
81	12.310	3501	3505	3506	rBV2	324	228	0.02%	0.002%
82	12.509	3565	3567	3569	rBV	353	184	0.02%	0.002%
83	12.651	3608	3611	3612	rBV2	306	192	0.02%	0.002%
84	12.699	3623	3626	3630	rBV4	476	339	0.03%	0.003%
85	12.802	3655	3658	3659	rBV4	517	267	0.02%	0.003%
86	12.831	3665	3667	3669	rBV2	411	200	0.02%	0.002%
87	12.882	3681	3683	3685	rBV	417	214	0.02%	0.002%
88	12.918	3690	3694	3703	rBV5	630	684	0.06%	0.007%
89	12.953	3703	3705	3707	rBV	321	144	0.01%	0.001%
90	13.114	3753	3755	3757	rBV2	415	211	0.02%	0.002%
91	13.198	3779	3781	3783	rBV2	364	201	0.02%	0.002%
92	13.281	3804	3807	3810	rBV2	321	245	0.02%	0.002%
93	13.342	3822	3826	3829	rVB3	539	342	0.03%	0.003%
94	13.362	3829	3832	3836	rBV3	507	473	0.04%	0.005%
95	13.423	3849	3851	3856	rBV2	348	217	0.02%	0.002%
96	13.616	3909	3911	3915	rBV	336	270	0.02%	0.003%
97	13.738	3947	3949	3953	rVB2	420	224	0.02%	0.002%
98	13.828	3975	3977	3978	rBV2	427	174	0.01%	0.002%
99	13.940	4011	4012	4015	rBV2	365	160	0.01%	0.002%
100	14.847	4292	4294	4299	rBV3	531	409	0.03%	0.004%

Sum of corrected areas: 10130597

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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



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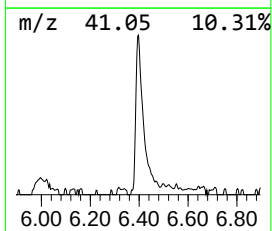
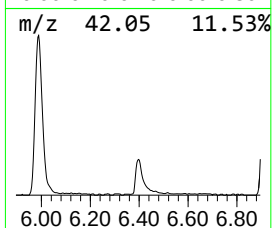
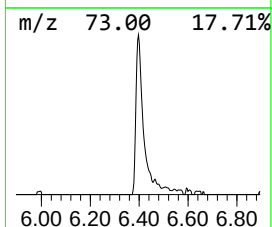
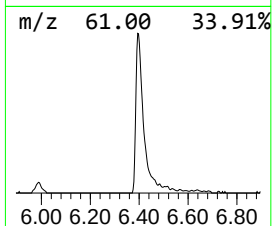
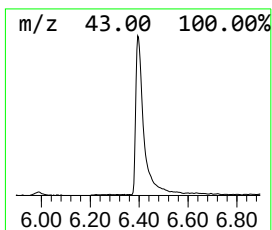
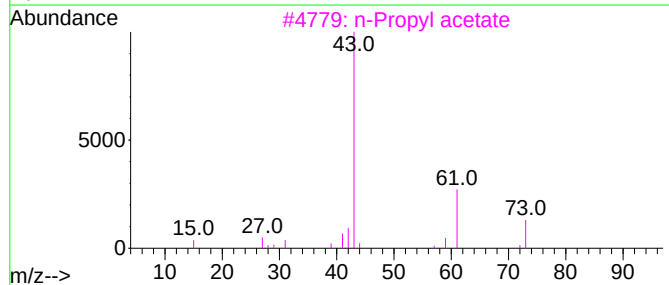
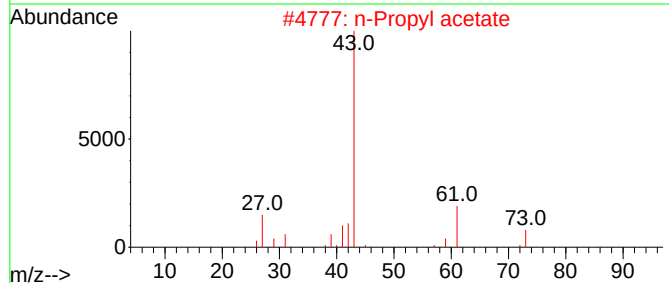
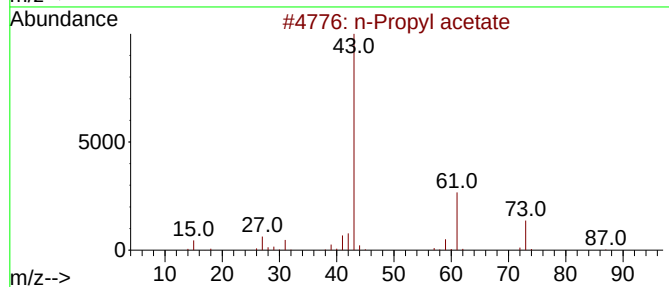
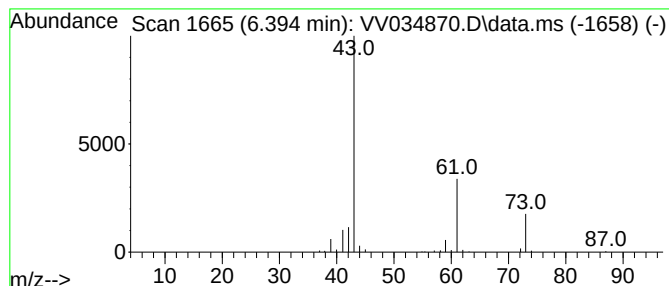
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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.
6.394	9.55 ug/L	149219	1,4-Difluorobenzene	5.532

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



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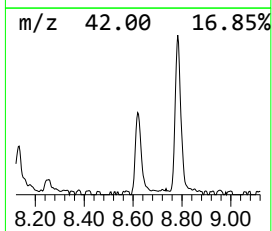
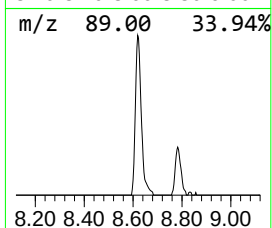
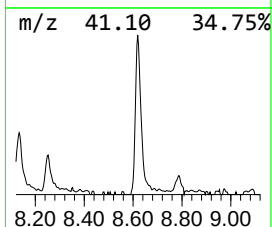
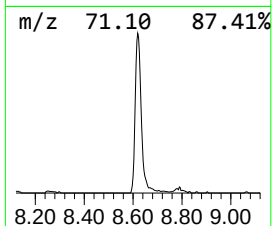
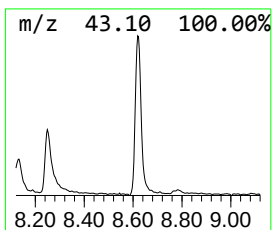
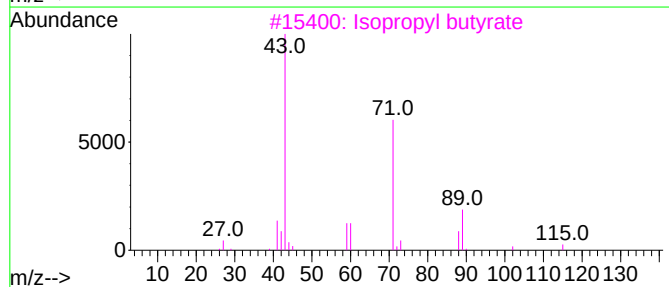
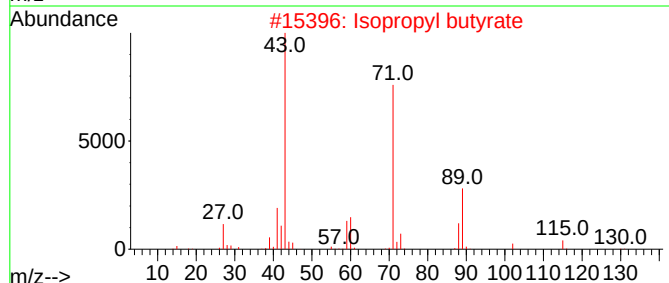
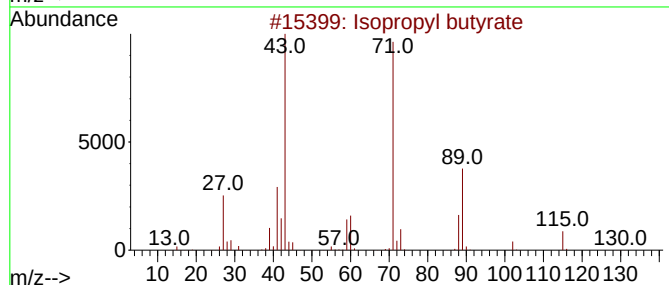
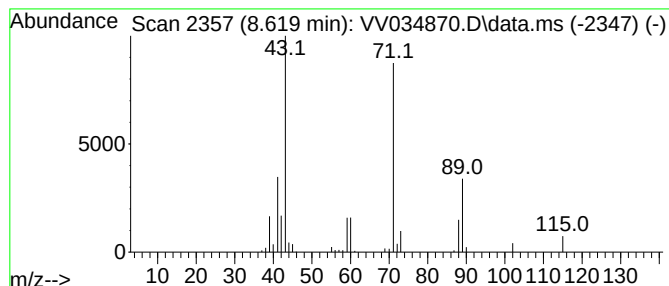
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Quant Title : VOC Analysis

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.
8.619	6.20 ug/L	123326	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
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 Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.394	9.6	ug/L	149219	1	5.532	781639	50.0
Isopropyl butyrate	8.619	6.2	ug/L	123326	2	8.783	994410	50.0