

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032124\
 Data File : VV034781.D
 Acq On : 21 Mar 2024 12:02
 Operator : SY/MD
 Sample : P1743-02 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E0737

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\SFAMVLM022924WMA.M
 Title : VOC Analysis

Signal : TIC: VV034781.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.281	68	75	91	rVB	243658	258868	16.79%	2.264%
2	1.532	146	153	171	rVB	204877	237768	15.42%	2.079%
3	2.060	307	317	331	rBV	335972	491346	31.87%	4.296%
4	2.240	370	373	379	rVB4	802	882	0.06%	0.008%
5	2.452	429	439	449	rVB2	6219	10614	0.69%	0.093%
6	2.519	456	460	463	rBV	249	266	0.02%	0.002%
7	2.568	473	475	478	rBV	215	120	0.01%	0.001%
8	2.590	480	482	483	rVV	229	96	0.01%	0.001%
9	2.616	487	490	492	rVB2	306	170	0.01%	0.001%
10	2.648	497	500	502	rBV2	256	137	0.01%	0.001%
11	2.703	515	517	520	rVB3	550	316	0.02%	0.003%
12	2.722	520	523	526	rVB2	140	100	0.01%	0.001%
13	2.838	556	559	564	rBV	121	139	0.01%	0.001%
14	2.899	571	578	581	rBV2	206	265	0.02%	0.002%
15	2.915	581	583	585	rBV2	229	102	0.01%	0.001%
16	3.024	612	617	620	rBV2	261	238	0.02%	0.002%
17	3.159	656	659	662	rVB2	157	96	0.01%	0.001%
18	3.182	662	666	669	rBV	158	105	0.01%	0.001%
19	3.207	669	674	678	rVB3	251	241	0.02%	0.002%
20	3.230	678	681	685	rVB2	172	150	0.01%	0.001%
21	3.278	693	696	700	rVB2	169	103	0.01%	0.001%
22	3.365	720	723	725	rBV2	147	110	0.01%	0.001%
23	3.519	767	771	775	rVB2	151	102	0.01%	0.001%
24	3.571	783	787	788	rBV2	221	89	0.01%	0.001%
25	3.587	790	792	796	rVB2	132	84	0.01%	0.001%
26	3.664	812	816	827	rVV4	671	1062	0.07%	0.009%
27	3.793	846	856	893	rBV	87936	262155	17.00%	2.292%
28	4.246	982	997	1035	rBV	237768	609095	39.51%	5.326%
29	4.629	1114	1116	1118	rBV	285	138	0.01%	0.001%
30	4.728	1144	1147	1148	rVV2	187	95	0.01%	0.001%
31	4.770	1158	1160	1161	rBV	198	86	0.01%	0.001%
32	4.828	1175	1178	1180	rBV2	254	176	0.01%	0.002%
33	4.844	1180	1183	1188	rBV3	274	300	0.02%	0.003%
34	4.883	1192	1195	1198	rVB2	326	230	0.01%	0.002%
35	4.957	1201	1218	1263	rBV2	576392	1541747	100.00%	13.481%
36	5.532	1386	1397	1430	rBV	390564	809738	52.52%	7.080%

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 Title : VOC Analysis

37	5.831	1480	1490	1505	rBV4	11130	25085	1.63%	0.219%
38	5.985	1526	1538	1568	rBV	324311	675625	43.82%	5.908%
39	6.301	1627	1636	1637	rBV6	2662	3334	0.22%	0.029%
40	6.397	1657	1666	1699	rBV	86926	185986	12.06%	1.626%
41	6.728	1767	1769	1774	rVB3	484	288	0.02%	0.003%
42	6.911	1816	1826	1859	rBV	180414	343979	22.31%	3.008%
43	7.120	1883	1891	1906	rBV	21378	38306	2.48%	0.335%
44	7.243	1918	1929	1953	rBV	686709	1216034	78.87%	10.633%
45	7.551	2016	2025	2055	rBV2	141949	273651	17.75%	2.393%
46	7.863	2112	2122	2139	rBV2	27270	49612	3.22%	0.434%
47	7.976	2149	2157	2162	rBV5	6906	10126	0.66%	0.089%
48	8.024	2163	2172	2198	rBV	292876	587435	38.10%	5.136%
49	8.249	2236	2242	2261	rVB2	19530	35269	2.29%	0.308%
50	8.548	2332	2335	2336	rBV	494	232	0.02%	0.002%
51	8.619	2347	2357	2379	rBV	78420	132280	8.58%	1.157%
52	8.783	2397	2408	2434	rBV	599325	995641	64.58%	8.706%
53	9.001	2474	2476	2478	rBV2	496	268	0.02%	0.002%
54	9.143	2519	2520	2522	rBV2	212	91	0.01%	0.001%
55	9.239	2546	2550	2554	rVB3	308	236	0.02%	0.002%
56	9.300	2566	2569	2573	rBV2	315	257	0.02%	0.002%
57	9.464	2617	2620	2621	rBV2	168	97	0.01%	0.001%
58	9.500	2623	2631	2641	rBV5	3772	6839	0.44%	0.060%
59	9.619	2666	2668	2674	rVB3	829	518	0.03%	0.005%
60	9.661	2678	2681	2683	rBV2	248	156	0.01%	0.001%
61	9.696	2690	2692	2693	rBV	362	152	0.01%	0.001%
62	9.802	2721	2725	2730	rVB2	186	143	0.01%	0.001%
63	9.857	2740	2742	2745	rBV2	160	112	0.01%	0.001%
64	10.005	2786	2788	2790	rBV	265	110	0.01%	0.001%
65	10.066	2800	2807	2810	rBV2	256	244	0.02%	0.002%
66	10.088	2812	2814	2817	rBV2	247	138	0.01%	0.001%
67	10.104	2817	2819	2821	rBV	241	114	0.01%	0.001%
68	10.149	2821	2833	2855	rBV	413745	649390	42.12%	5.678%
69	10.326	2885	2888	2893	rVB	881	589	0.04%	0.005%
70	10.365	2898	2900	2903	rBV2	115	79	0.01%	0.001%
71	10.384	2903	2906	2908	rBV	179	87	0.01%	0.001%
72	10.448	2922	2926	2929	rBV	208	186	0.01%	0.002%
73	10.551	2955	2958	2964	rBV	326	234	0.02%	0.002%
74	10.635	2982	2984	2987	rVB2	254	97	0.01%	0.001%
75	10.677	2993	2997	3001	rBV	279	249	0.02%	0.002%
76	10.699	3001	3004	3012	rVB	235	307	0.02%	0.003%

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77	10.821	3039	3042	3044	rBV	171	111	0.01%	0.001%
78	10.857	3052	3053	3056	rVB2	381	145	0.01%	0.001%
79	10.879	3056	3060	3064	rBV3	365	333	0.02%	0.003%
80	10.943	3077	3080	3084	rBV2	262	240	0.02%	0.002%
81	10.992	3092	3095	3097	rBV2	212	146	0.01%	0.001%
82	11.062	3115	3117	3123	rVB2	240	152	0.01%	0.001%
83	11.133	3134	3139	3144	rBV3	653	656	0.04%	0.006%
84	11.185	3144	3155	3181	rBV	596330	923417	59.89%	8.074%
85	11.493	3248	3251	3252	rBV	241	123	0.01%	0.001%
86	11.558	3260	3271	3291	rBV	661091	1045424	67.81%	9.141%
87	12.406	3533	3535	3537	rBV	277	95	0.01%	0.001%
88	12.448	3546	3548	3552	rVB	344	181	0.01%	0.002%
89	12.532	3571	3574	3577	rBV2	402	276	0.02%	0.002%
90	12.609	3594	3598	3601	rBV2	518	340	0.02%	0.003%
91	12.857	3672	3675	3678	rBV	347	244	0.02%	0.002%
92	13.120	3755	3757	3758	rBV	254	113	0.01%	0.001%
93	13.188	3775	3778	3781	rBV2	361	254	0.02%	0.002%
94	13.213	3781	3786	3794	rVB3	705	940	0.06%	0.008%
95	13.686	3930	3933	3948	rVB5	1031	1477	0.10%	0.013%
96	13.792	3964	3966	3968	rBV2	409	168	0.01%	0.001%
97	13.969	4018	4021	4022	rBV	399	204	0.01%	0.002%
98	14.072	4050	4053	4054	rBV	328	215	0.01%	0.002%
99	14.104	4061	4063	4064	rBV	410	135	0.01%	0.001%
100	14.930	4317	4320	4321	rBV	518	279	0.02%	0.002%

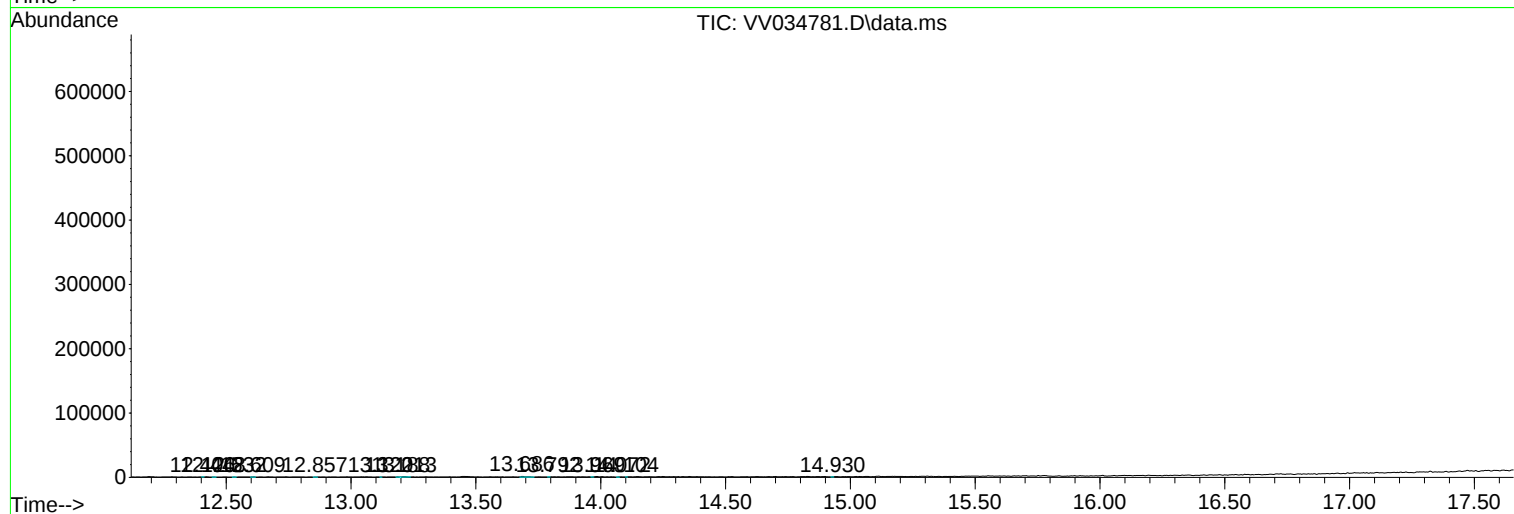
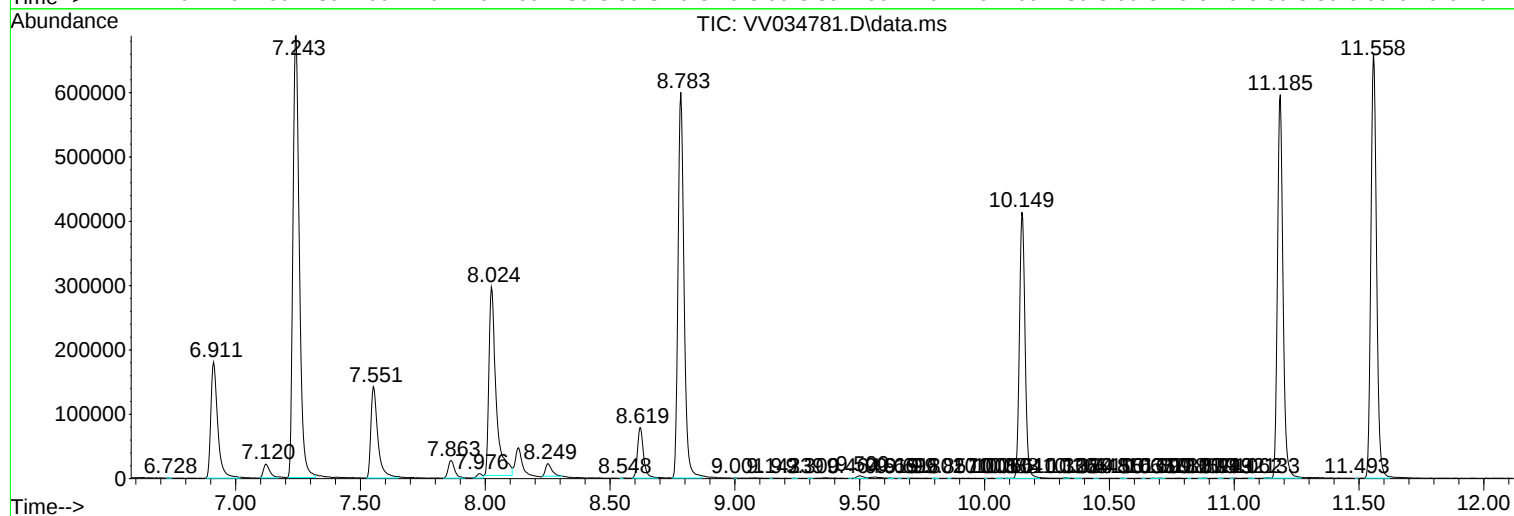
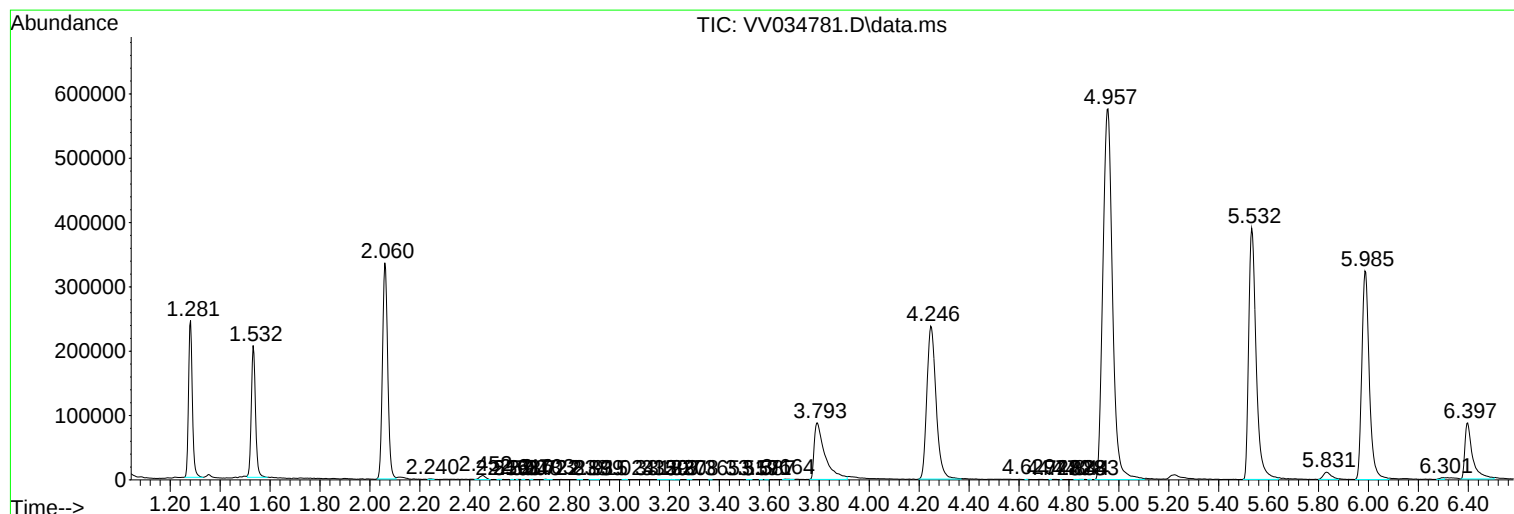
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022924WMA.M
Quant Title : VOC Analysis

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



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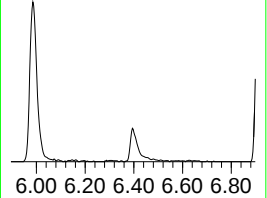
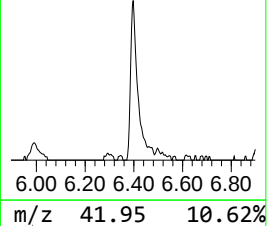
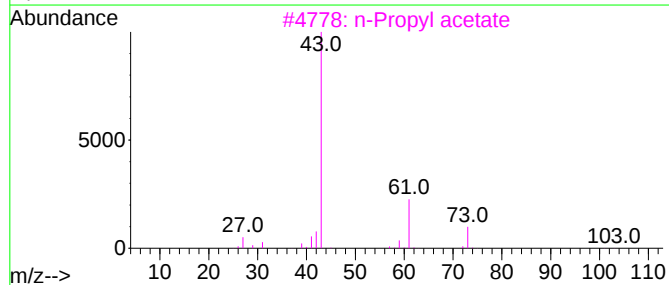
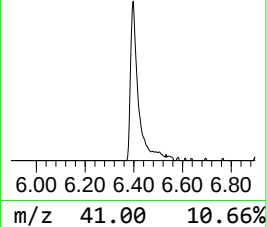
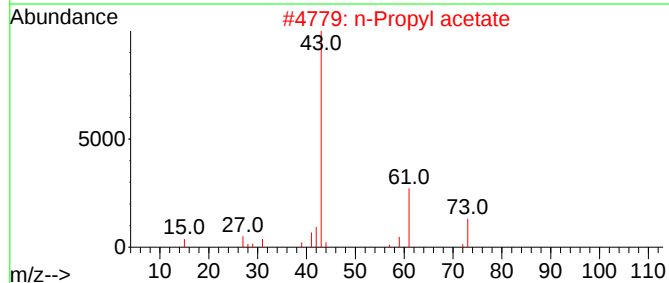
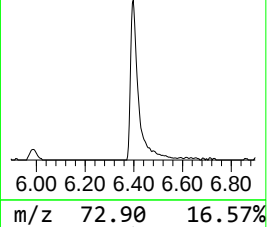
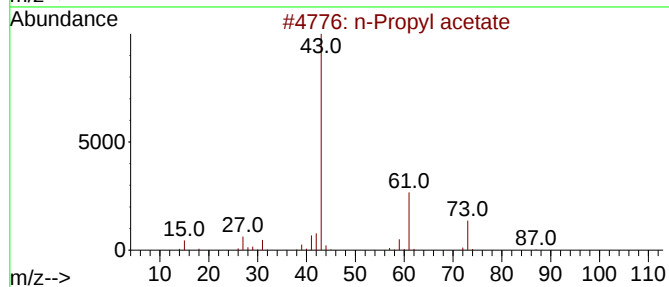
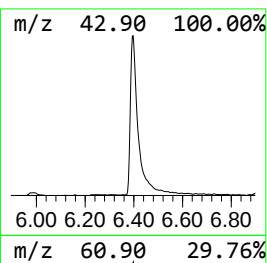
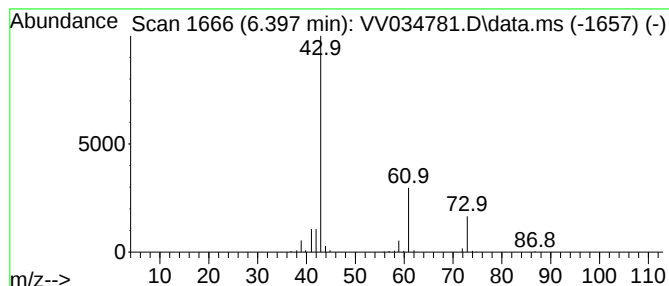
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022924WMA.M
Quant Title : VOC Analysis

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.
6.397	11.48 ug/L	185986	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	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	72



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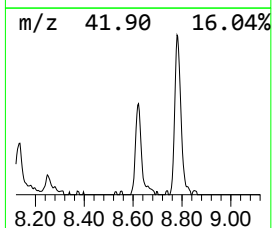
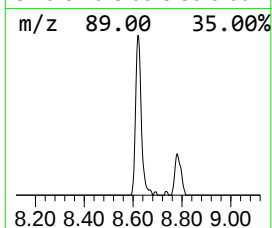
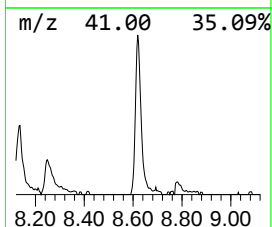
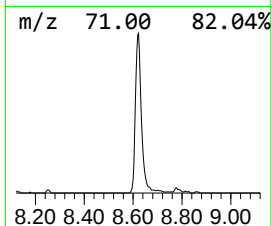
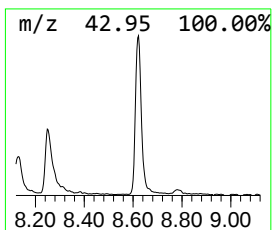
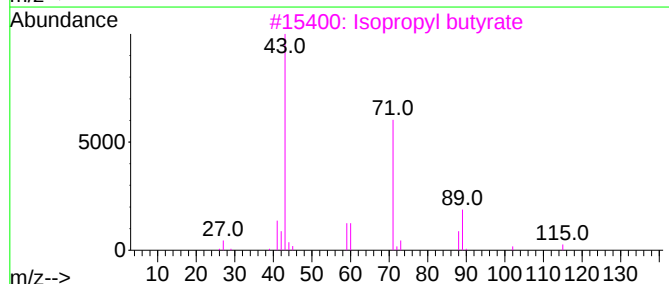
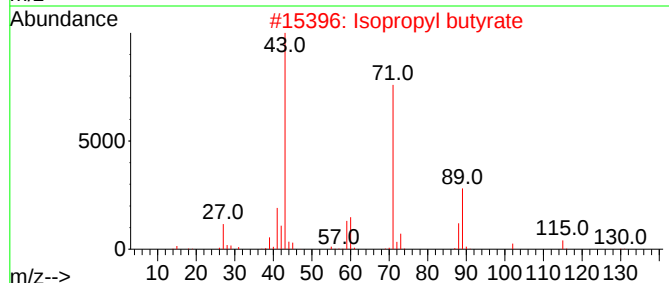
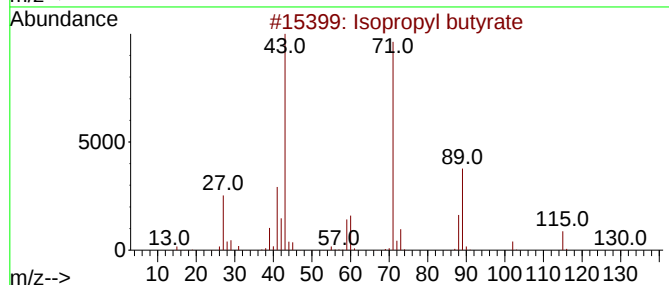
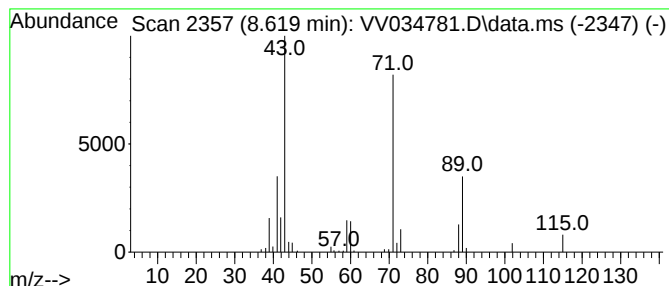
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Quant Title : VOC Analysis

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	6.64 ug/L	132280	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	83
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	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	6.397	11.5	ug/L	185986	1	5.532	809738	50.0
Isopropyl butyrate	8.619	6.6	ug/L	132280	2	8.783	995641	50.0