

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032724\
 Data File : VV034860.D
 Acq On : 27 Mar 2024 13:17
 Operator : SY/MD
 Sample : PB159798TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 9 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: VV034860.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	92	rVB	160477	177614	13.53%	1.635%
2	1.526	146	151	166	rVB	140156	156830	11.94%	1.443%
3	2.056	306	316	329	rBV	297747	435616	33.18%	4.009%
4	2.555	461	471	486	rBV3	4988	11261	0.86%	0.104%
5	2.732	525	526	528	rBV	237	99	0.01%	0.001%
6	2.744	528	530	532	rVV3	372	179	0.01%	0.002%
7	2.777	537	540	545	rBV	366	335	0.03%	0.003%
8	2.860	563	566	568	rBV2	449	304	0.02%	0.003%
9	2.902	575	579	583	rVV3	512	387	0.03%	0.004%
10	2.918	583	584	585	rVB	356	69	0.01%	0.001%
11	3.034	618	620	621	rVB	301	101	0.01%	0.001%
12	3.043	621	623	629	rBV2	366	367	0.03%	0.003%
13	3.079	631	634	635	rBV	193	120	0.01%	0.001%
14	3.114	636	645	648	rBV4	3251	4653	0.35%	0.043%
15	3.275	692	695	698	rBV3	373	260	0.02%	0.002%
16	3.339	713	715	718	rBV2	325	231	0.02%	0.002%
17	3.375	725	726	728	rBV2	129	70	0.01%	0.001%
18	3.426	740	742	743	rBV	156	60	0.00%	0.001%
19	3.445	745	748	750	rVV2	537	328	0.02%	0.003%
20	3.474	754	757	760	rVB2	232	132	0.01%	0.001%
21	3.558	781	783	788	rVB3	396	288	0.02%	0.003%
22	3.587	788	792	793	rBV	319	173	0.01%	0.002%
23	3.596	793	795	800	rVB3	448	359	0.03%	0.003%
24	3.699	824	827	829	rBV	179	107	0.01%	0.001%
25	3.796	847	857	908	rBV	88084	298442	22.73%	2.747%
26	4.246	983	997	1029	rBV	211698	538089	40.98%	4.952%
27	4.616	1110	1112	1113	rBV2	362	164	0.01%	0.002%
28	4.635	1116	1118	1120	rVB	403	159	0.01%	0.001%
29	4.686	1132	1134	1136	rBV2	345	141	0.01%	0.001%
30	4.831	1175	1179	1182	rVB3	325	268	0.02%	0.002%
31	4.850	1183	1185	1186	rBV	274	101	0.01%	0.001%
32	4.886	1195	1196	1198	rVB	201	55	0.00%	0.001%
33	4.953	1202	1217	1250	rBV2	498654	1313012	100.00%	12.085%
34	5.532	1386	1397	1433	rBV	417744	868823	66.17%	7.996%
35	5.834	1481	1491	1502	rBV3	9852	21336	1.62%	0.196%
36	5.985	1526	1538	1566	rBV	294710	614197	46.78%	5.653%

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 Title : VOC Analysis

37	6.397	1658	1666	1706	rBV	82197	179734	13.69%	1.654%
38	6.876	1810	1815	1816	rBV2	853	673	0.05%	0.006%
39	6.911	1816	1826	1851	rVV	158637	302149	23.01%	2.781%
40	7.124	1884	1892	1916	rBV	20418	40198	3.06%	0.370%
41	7.243	1918	1929	1958	rBV	543206	966238	73.59%	8.893%
42	7.554	2016	2026	2051	rBV2	129950	252457	19.23%	2.324%
43	7.863	2113	2122	2137	rBV2	29347	51220	3.90%	0.471%
44	8.030	2165	2174	2199	rBV	295093	628759	47.89%	5.787%
45	8.252	2236	2243	2261	rBV	21103	40167	3.06%	0.370%
46	8.506	2319	2322	2324	rBV2	673	401	0.03%	0.004%
47	8.622	2348	2358	2381	rBV	86584	145480	11.08%	1.339%
48	8.783	2397	2408	2446	rBV	658544	1092670	83.22%	10.057%
49	9.001	2472	2476	2479	rBV4	715	632	0.05%	0.006%
50	9.326	2574	2577	2578	rBV2	451	298	0.02%	0.003%
51	9.503	2623	2632	2646	rBV9	3972	9191	0.70%	0.085%
52	9.841	2733	2737	2740	rVB2	522	363	0.03%	0.003%
53	9.898	2753	2755	2758	rVB3	303	131	0.01%	0.001%
54	9.937	2763	2767	2771	rVB2	335	251	0.02%	0.002%
55	9.960	2771	2774	2777	rBV	444	351	0.03%	0.003%
56	10.152	2821	2834	2864	rBV	448084	719917	54.83%	6.626%
57	10.403	2910	2912	2913	rBV	366	165	0.01%	0.002%
58	10.484	2929	2937	2938	rBV5	873	1022	0.08%	0.009%
59	10.648	2987	2988	2991	rVB2	352	119	0.01%	0.001%
60	10.673	2994	2996	3001	rVB3	409	231	0.02%	0.002%
61	10.841	3046	3048	3049	rBV	427	177	0.01%	0.002%
62	10.921	3069	3073	3076	rBV3	480	480	0.04%	0.004%
63	11.050	3110	3113	3115	rBV3	354	233	0.02%	0.002%
64	11.098	3125	3128	3130	rBV	320	175	0.01%	0.002%
65	11.107	3130	3131	3133	rBV	224	88	0.01%	0.001%
66	11.140	3134	3141	3144	rBV5	1052	1110	0.08%	0.010%
67	11.185	3144	3155	3178	rBV	660185	1030464	78.48%	9.484%
68	11.439	3232	3234	3235	rBV	270	112	0.01%	0.001%
69	11.561	3260	3272	3295	rBV	590808	949498	72.31%	8.739%
70	11.828	3351	3355	3358	rBV3	658	668	0.05%	0.006%
71	11.924	3383	3385	3391	rBV3	449	446	0.03%	0.004%
72	12.104	3439	3441	3445	rBV3	390	219	0.02%	0.002%
73	12.159	3456	3458	3460	rBV3	407	187	0.01%	0.002%
74	12.255	3486	3488	3491	rBV	352	185	0.01%	0.002%
75	12.696	3622	3625	3627	rBV2	463	279	0.02%	0.003%
76	12.786	3650	3653	3654	rBV	410	234	0.02%	0.002%

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Title : VOC Analysis

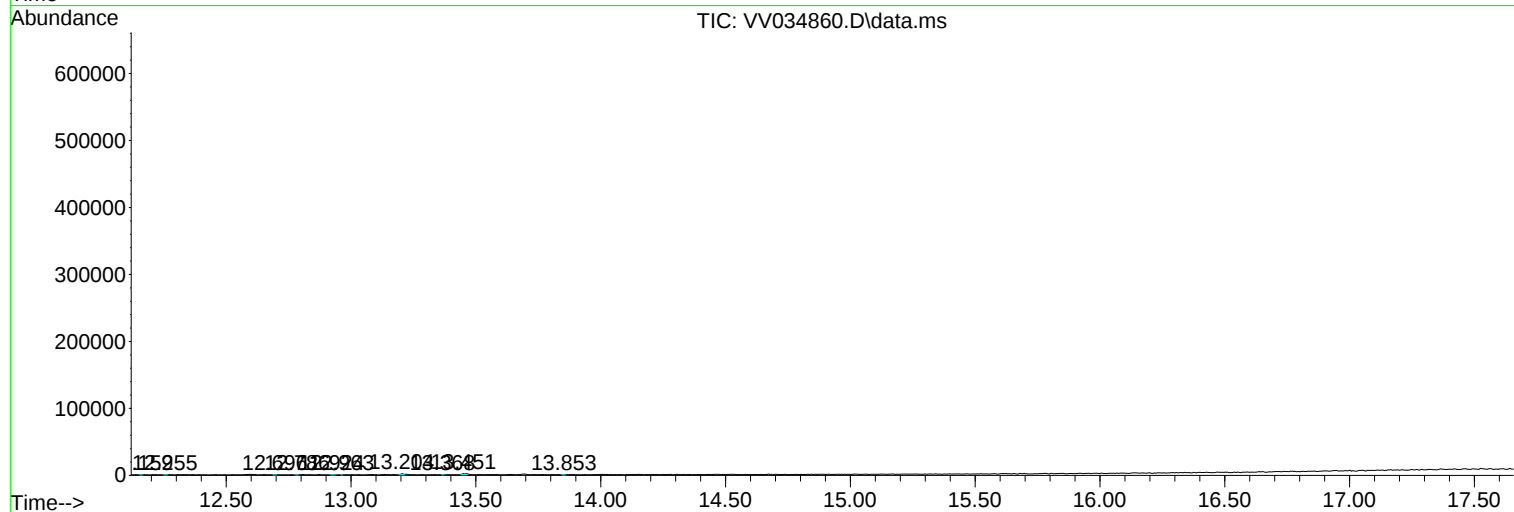
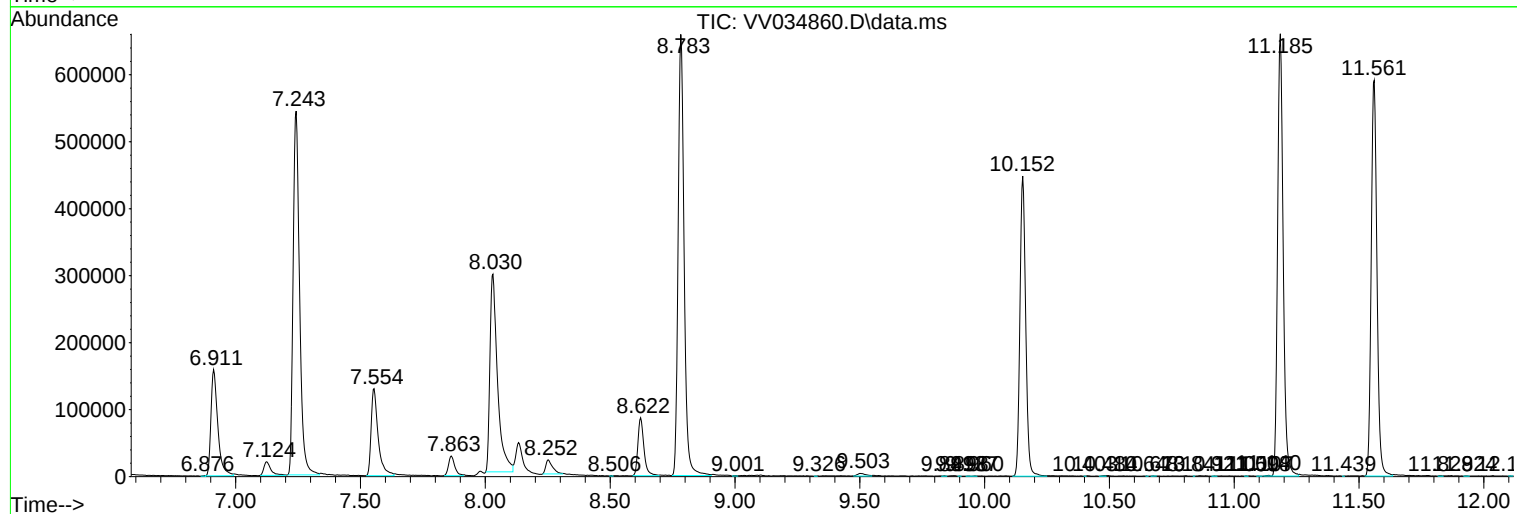
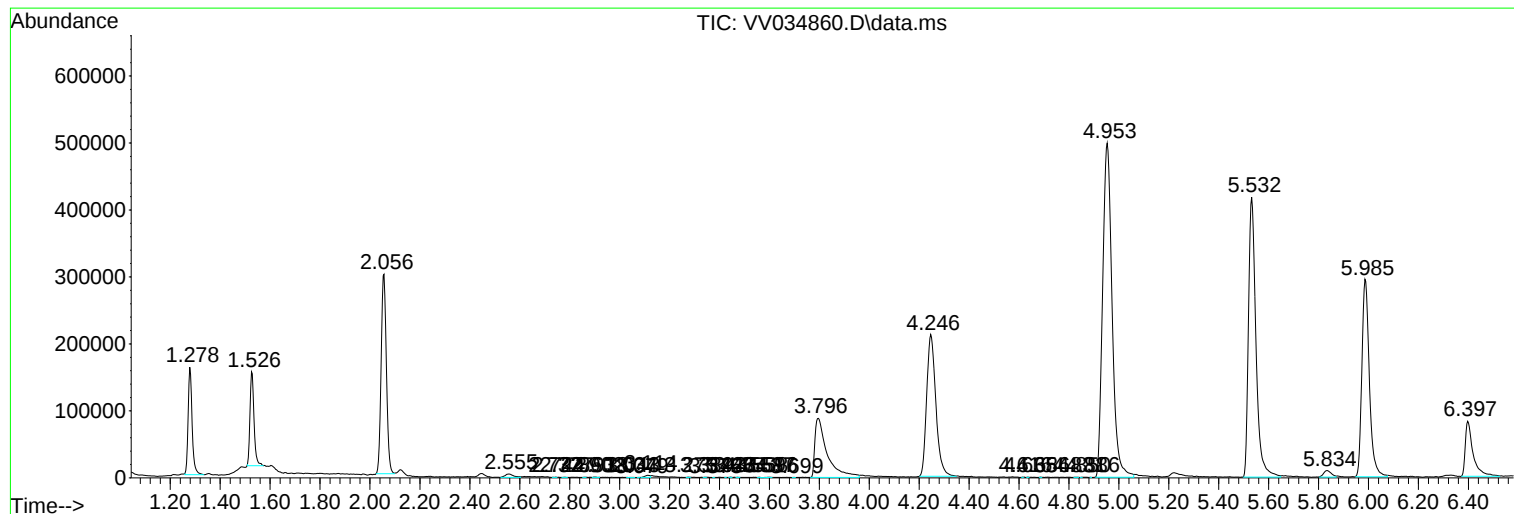
77	12.924	3694	3696	3700	rBV2	325	220	0.02%	0.002%
78	12.963	3707	3708	3709	rBV2	252	91	0.01%	0.001%
79	13.204	3779	3783	3786	rBV3	1497	1298	0.10%	0.012%
80	13.368	3832	3834	3836	rBV2	415	135	0.01%	0.001%
81	13.451	3856	3860	3862	rBV3	1398	1108	0.08%	0.010%
82	13.853	3982	3985	3987	rBV2	382	248	0.02%	0.002%

Sum of corrected areas: 10865202

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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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ALS Vial : 9 Sample Multiplier: 1

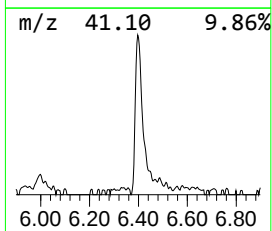
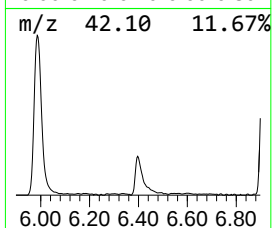
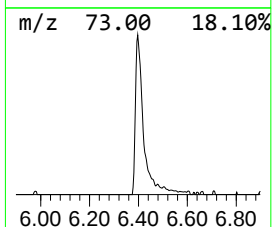
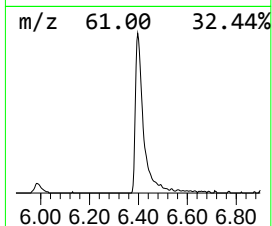
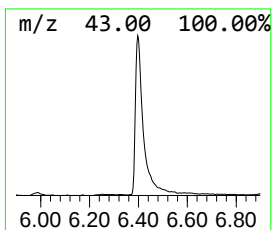
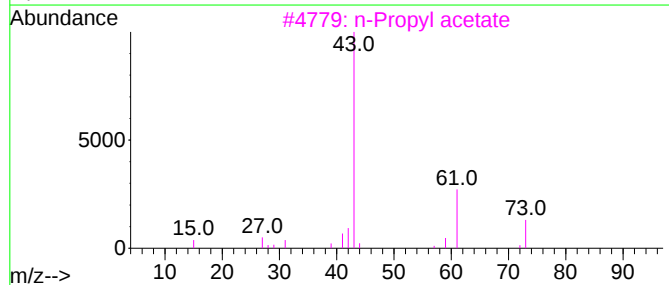
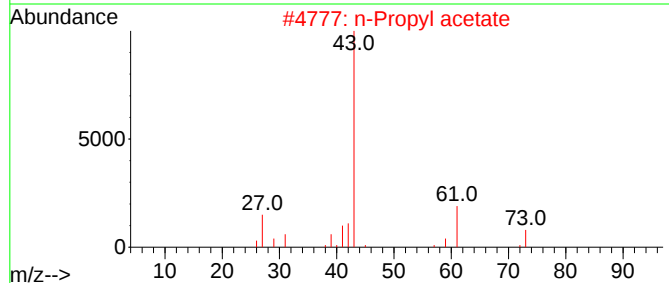
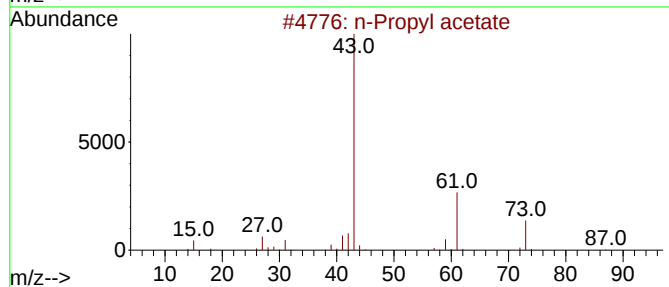
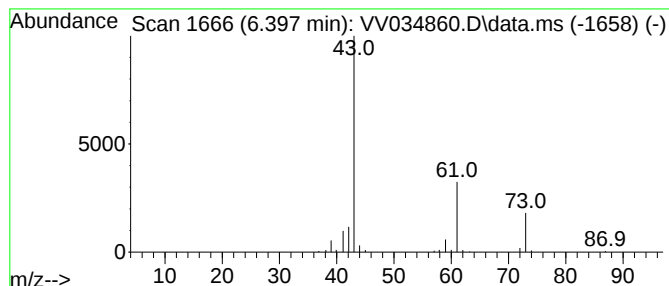
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM032624WMA.M
Quant Title : VOC Analysis

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.
6.397	10.34 ug/L	179734	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	72
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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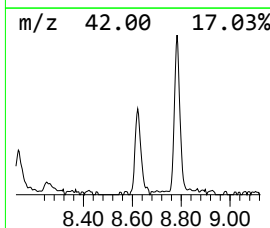
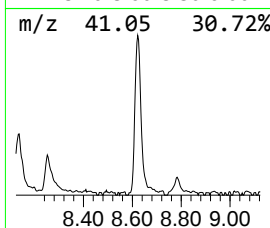
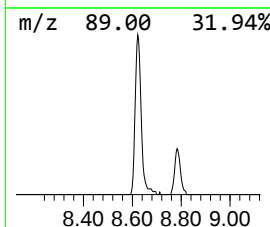
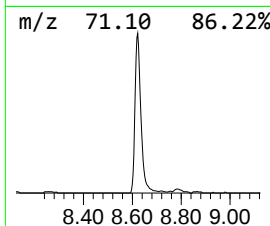
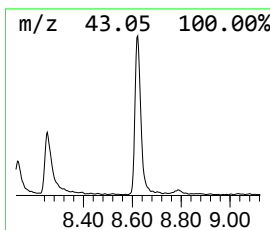
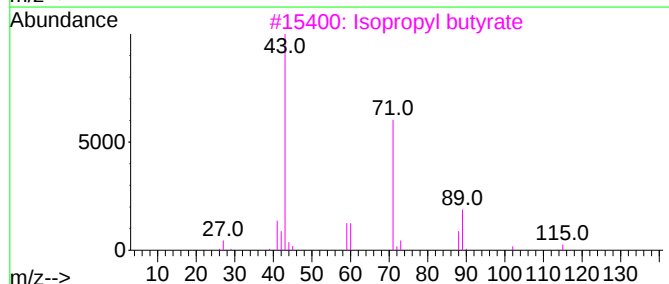
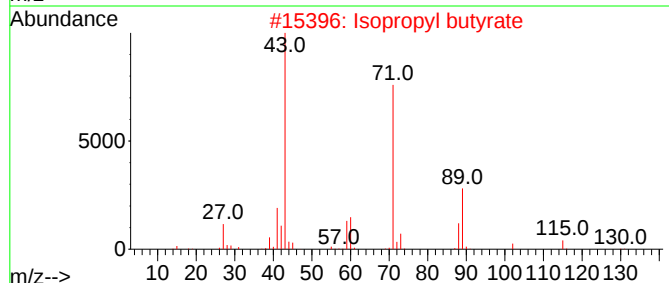
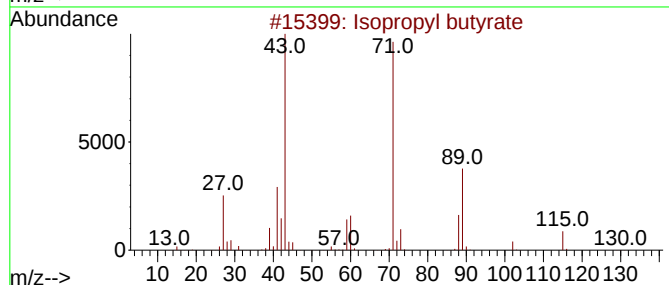
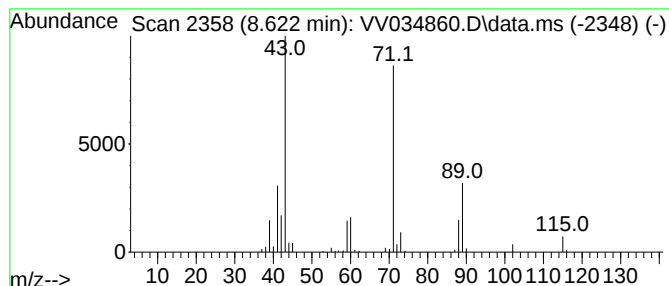
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.622	6.66 ug/L	145480	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			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64



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Quant Title : VOC Analysis

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	10.3	ug/L	179734	1	5.532	868823	50.0
Isopropyl butyrate	8.622	6.7	ug/L	145480	2	8.783	1092670	50.0