

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
 Data File : VU055772.D
 Acq On : 16 Oct 2023 15:12
 Operator : MD/SY
 Sample : 04874-02 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COM26

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: VU055772.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	114	rBV	223053	265229	13.44%	1.763%
2	1.888	178	186	203	rVB	186564	270279	13.69%	1.797%
3	2.557	382	394	409	rBV	386094	634100	32.12%	4.215%
4	2.782	460	464	468	rBV3	946	928	0.05%	0.006%
5	2.849	481	485	488	rBV3	652	427	0.02%	0.003%
6	2.882	491	495	498	rVB2	442	292	0.01%	0.002%
7	2.939	510	513	518	rBV3	453	382	0.02%	0.003%
8	3.036	533	543	557	rVB2	10274	19265	0.98%	0.128%
9	3.177	572	587	588	rBV4	6103	8460	0.43%	0.056%
10	3.422	657	663	665	rBV	285	269	0.01%	0.002%
11	3.502	685	688	693	rVB2	363	329	0.02%	0.002%
12	3.576	705	711	716	rBV2	591	536	0.03%	0.004%
13	3.689	742	746	752	rVV2	529	460	0.02%	0.003%
14	3.891	806	809	813	rVB	559	399	0.02%	0.003%
15	3.917	813	817	819	rBV2	393	258	0.01%	0.002%
16	3.933	819	822	826	rVV2	411	393	0.02%	0.003%
17	4.033	848	853	858	rVB	268	271	0.01%	0.002%
18	4.097	870	873	876	rBV2	437	310	0.02%	0.002%
19	4.290	927	933	936	rBV3	388	294	0.01%	0.002%
20	4.489	989	995	997	rBV3	321	282	0.01%	0.002%
21	4.615	1023	1034	1073	rBV	131961	366832	18.58%	2.438%
22	4.946	1133	1137	1142	rBV3	631	526	0.03%	0.003%
23	5.055	1155	1171	1204	rVV	357514	801091	40.58%	5.325%
24	5.251	1227	1232	1238	rVB5	575	640	0.03%	0.004%
25	5.328	1254	1256	1262	rVB3	578	498	0.03%	0.003%
26	5.608	1338	1343	1347	rBV2	272	316	0.02%	0.002%
27	5.717	1352	1377	1400	rBV2	716289	1974042	100.00%	13.122%
28	5.910	1429	1437	1450	rBV3	7482	14696	0.74%	0.098%
29	6.026	1471	1473	1476	rVB2	404	247	0.01%	0.002%
30	6.113	1497	1500	1502	rBV2	433	285	0.01%	0.002%
31	6.187	1518	1523	1526	rBV2	530	638	0.03%	0.004%
32	6.242	1527	1540	1576	rBV	533605	1040642	52.72%	6.918%
33	6.528	1617	1629	1644	rBV2	21401	41963	2.13%	0.279%
34	6.586	1644	1647	1651	rBV2	769	568	0.03%	0.004%
35	6.685	1663	1678	1706	rBV	451252	899074	45.54%	5.976%
36	6.926	1742	1753	1771	rBV2	5870	16046	0.81%	0.107%

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 Title : VOC Analysis

37	7.039	1777	1788	1811	rBV	63056	119421	6.05%	0.794%
38	7.187	1824	1834	1848	rBV5	7130	14207	0.72%	0.094%
39	7.338	1879	1881	1885	rBV3	438	318	0.02%	0.002%
40	7.454	1914	1917	1920	rVB2	391	303	0.02%	0.002%
41	7.492	1923	1929	1930	rBV2	438	422	0.02%	0.003%
42	7.560	1937	1950	1972	rBV	237409	430769	21.82%	2.863%
43	7.695	1985	1992	1994	rBV5	3308	3546	0.18%	0.024%
44	7.737	1997	2005	2017	rVB2	27123	44784	2.27%	0.298%
45	7.894	2041	2054	2079	rBV	868921	1529274	77.47%	10.166%
46	8.129	2122	2127	2129	rBV2	694	595	0.03%	0.004%
47	8.177	2129	2142	2169	rVV	168727	303316	15.37%	2.016%
48	8.293	2176	2178	2184	rVB4	1029	717	0.04%	0.005%
49	8.325	2184	2188	2192	rBV3	482	429	0.02%	0.003%
50	8.460	2217	2230	2244	rBV	32001	55194	2.80%	0.367%
51	8.573	2252	2265	2272	rBV9	5715	12721	0.64%	0.085%
52	8.634	2273	2284	2306	rBV3	365428	864391	43.79%	5.746%
53	8.840	2340	2348	2364	rVB2	9744	17714	0.90%	0.118%
54	8.984	2391	2393	2395	rBV2	441	244	0.01%	0.002%
55	9.032	2402	2408	2412	rBV4	755	797	0.04%	0.005%
56	9.052	2412	2414	2419	rVB	494	310	0.02%	0.002%
57	9.090	2422	2426	2429	rVB2	471	285	0.01%	0.002%
58	9.106	2429	2431	2435	rVB	390	262	0.01%	0.002%
59	9.145	2438	2443	2446	rVB	378	304	0.02%	0.002%
60	9.209	2449	2463	2478	rBV2	83622	141402	7.16%	0.940%
61	9.293	2487	2489	2492	rVB2	633	309	0.02%	0.002%
62	9.415	2514	2527	2548	rBV	788813	1318521	66.79%	8.765%
63	9.634	2591	2595	2596	rBV	491	311	0.02%	0.002%
64	9.692	2608	2613	2614	rBV3	947	711	0.04%	0.005%
65	9.730	2622	2625	2629	rVB2	592	402	0.02%	0.003%
66	9.843	2656	2660	2667	rVB4	418	471	0.02%	0.003%
67	9.923	2679	2685	2686	rBV3	1077	881	0.04%	0.006%
68	9.952	2692	2694	2700	rVB4	736	577	0.03%	0.004%
69	10.081	2722	2734	2742	rBV5	2670	5151	0.26%	0.034%
70	10.142	2750	2753	2756	rVB3	377	259	0.01%	0.002%
71	10.283	2795	2797	2801	rVB2	492	324	0.02%	0.002%
72	10.335	2808	2813	2814	rBV2	477	375	0.02%	0.002%
73	10.360	2817	2821	2826	rVB	436	331	0.02%	0.002%
74	10.483	2856	2859	2863	rBV	403	303	0.02%	0.002%
75	10.573	2884	2887	2893	rVB2	496	497	0.03%	0.003%
76	10.618	2893	2901	2905	rBV2	673	773	0.04%	0.005%

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77	10.753	2929	2943	2964	rBV	658720	1078501	54.63%	7.169%
78	10.942	3000	3002	3006	rVB	679	357	0.02%	0.002%
79	11.010	3021	3023	3026	rVB	507	266	0.01%	0.002%
80	11.029	3026	3029	3035	rBV3	380	297	0.02%	0.002%
81	11.129	3055	3060	3062	rBV2	664	570	0.03%	0.004%
82	11.290	3105	3110	3113	rBV	553	475	0.02%	0.003%
83	11.415	3147	3149	3154	rVB3	727	515	0.03%	0.003%
84	11.447	3154	3159	3162	rBV	543	463	0.02%	0.003%
85	11.547	3187	3190	3196	rVB2	438	431	0.02%	0.003%
86	11.585	3196	3202	3206	rBV2	659	809	0.04%	0.005%
87	11.605	3206	3208	3216	rVB2	271	340	0.02%	0.002%
88	11.810	3259	3272	3294	rBV	773399	1275845	64.63%	8.481%
89	12.138	3371	3374	3376	rBV2	628	329	0.02%	0.002%
90	12.190	3376	3390	3419	rBV	869786	1445359	73.22%	9.608%
91	12.595	3513	3516	3518	rBV	475	383	0.02%	0.003%
92	12.637	3525	3529	3531	rBV4	414	338	0.02%	0.002%
93	12.675	3539	3541	3543	rBV	499	279	0.01%	0.002%
94	12.762	3564	3568	3570	rBV3	698	559	0.03%	0.004%
95	13.119	3677	3679	3686	rVB4	878	818	0.04%	0.005%
96	13.254	3717	3721	3727	rBV3	510	629	0.03%	0.004%
97	13.441	3776	3779	3784	rBV3	426	328	0.02%	0.002%
98	13.801	3885	3891	3894	rBV2	1079	959	0.05%	0.006%
99	13.871	3910	3913	3919	rBV6	603	632	0.03%	0.004%
100	15.254	4339	4343	4347	rBV3	809	896	0.05%	0.006%

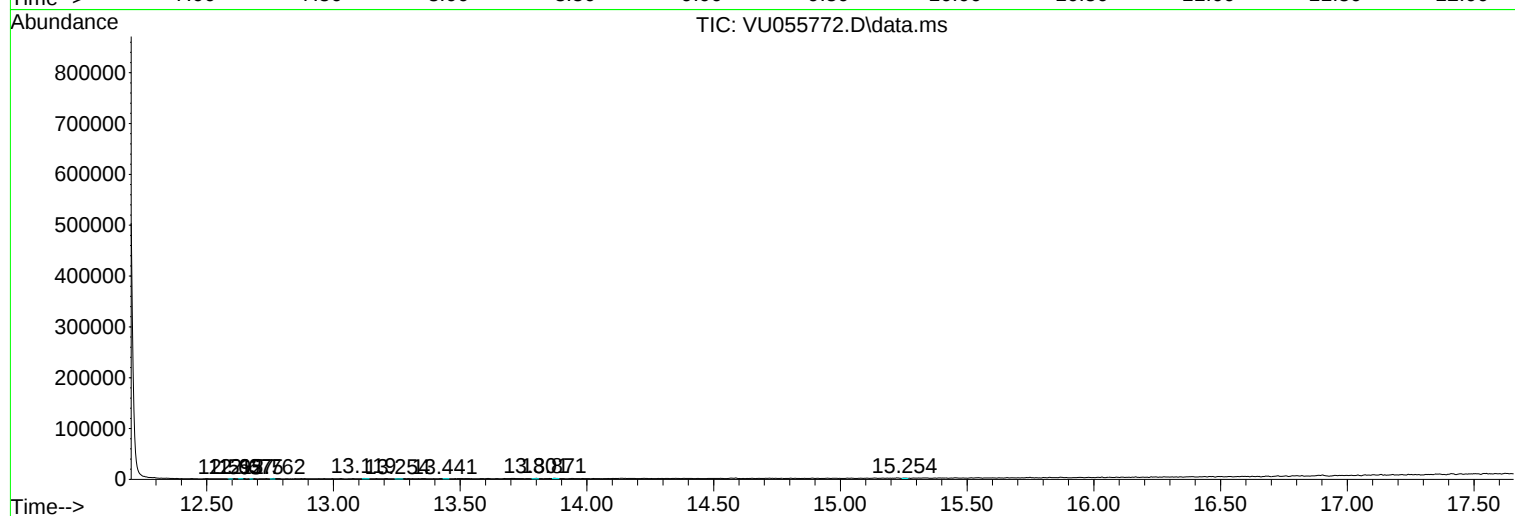
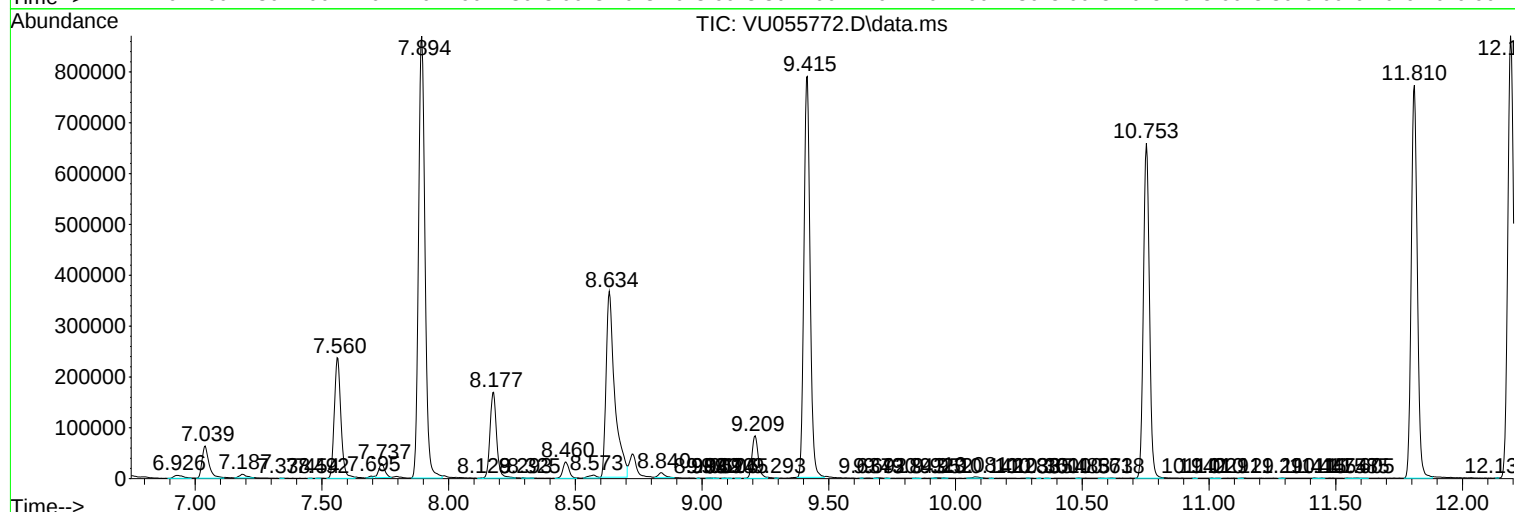
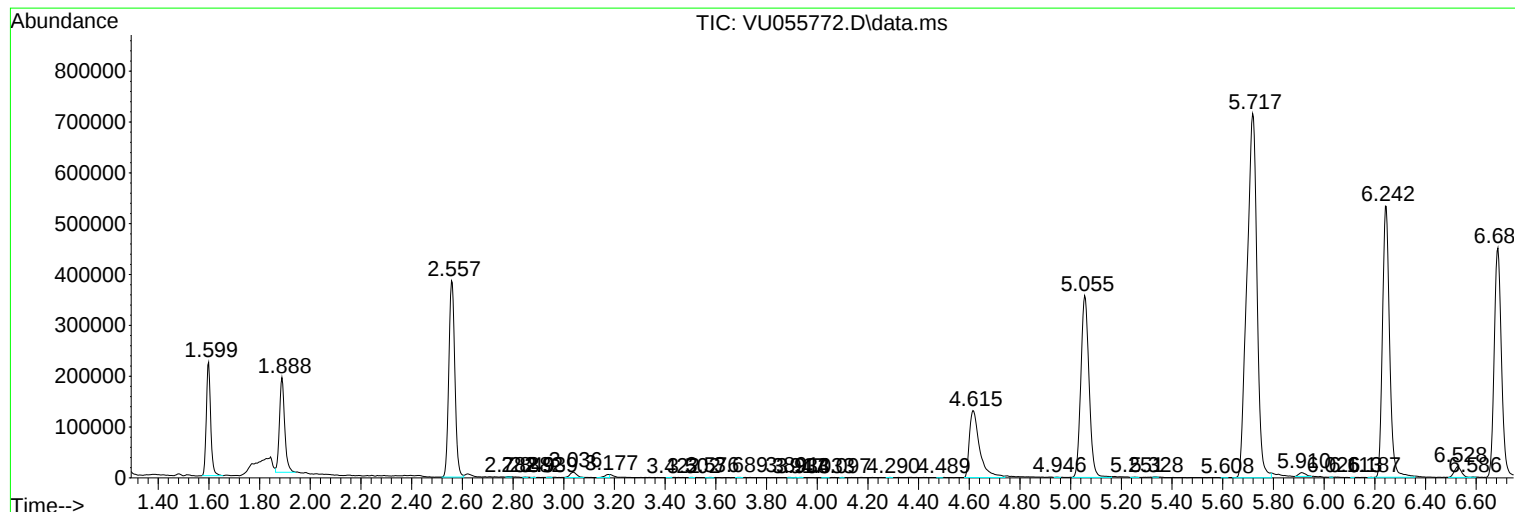
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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



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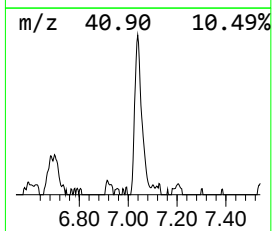
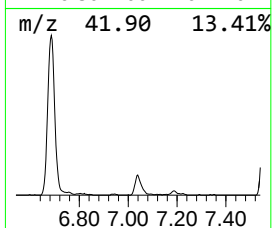
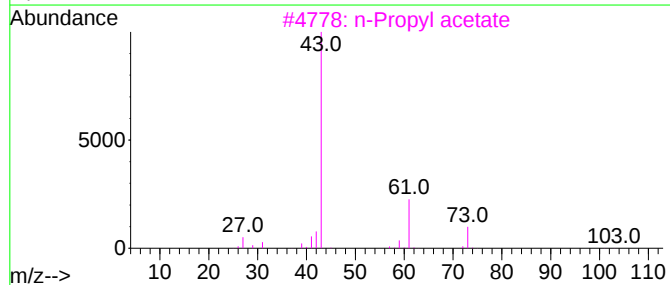
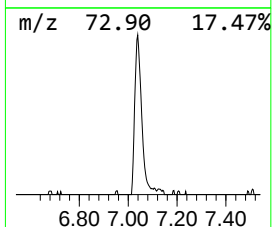
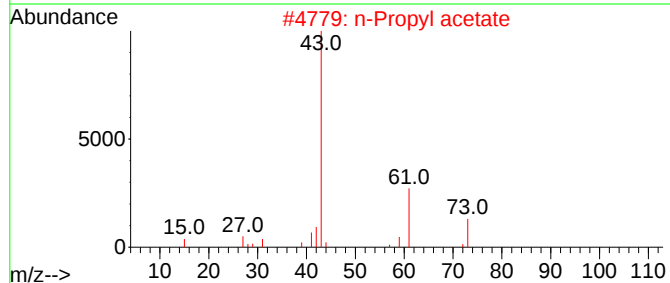
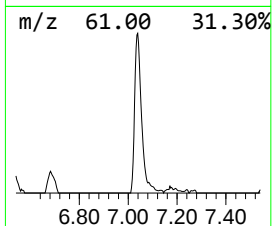
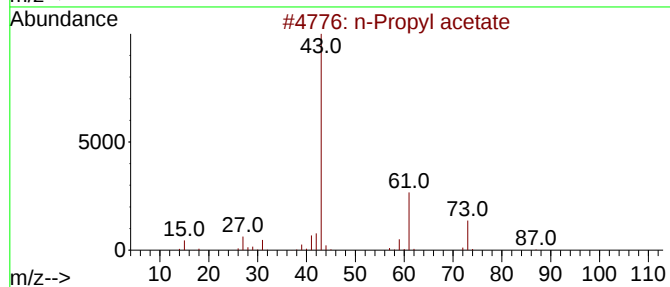
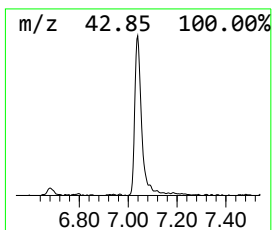
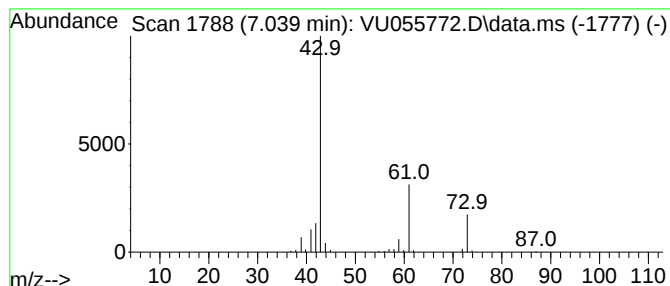
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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	5.74 ug/L	119421	1,4-Difluorobenzene	6.245

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	56



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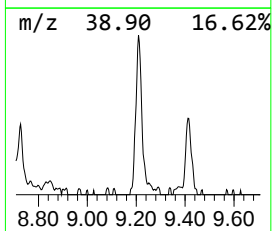
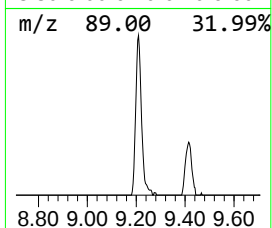
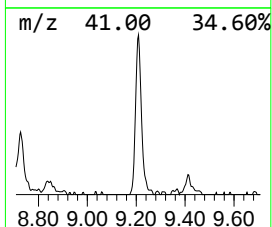
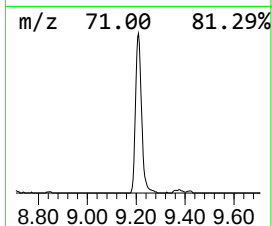
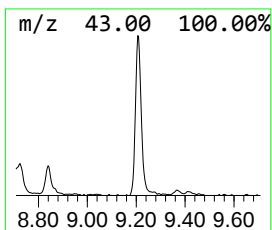
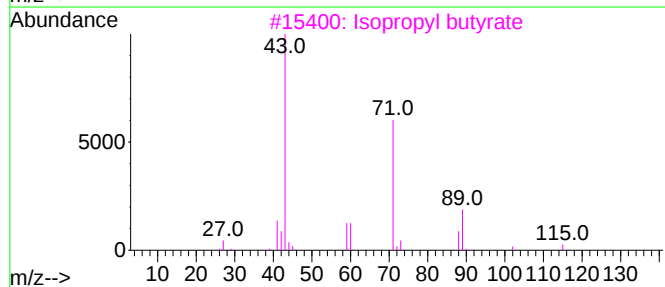
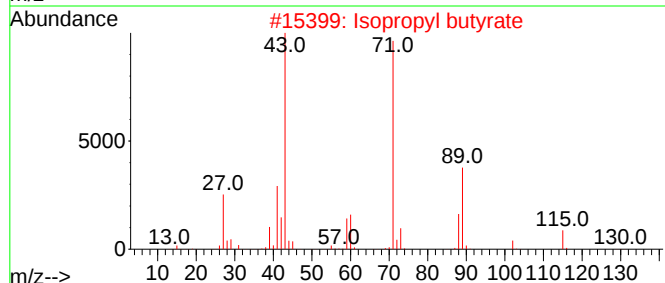
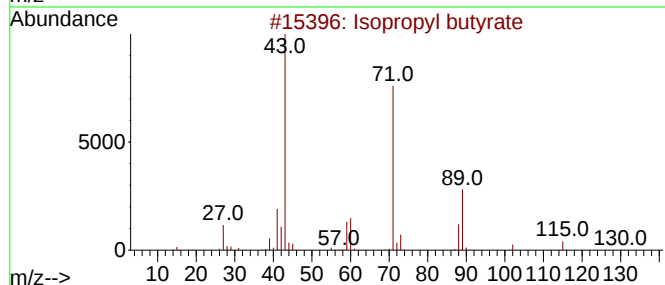
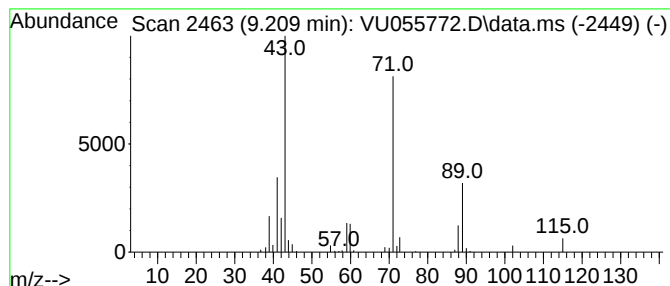
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.209	5.36 ug/L	141402	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			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



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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	7.039	5.7	ug/L	119421	1	6.245	1040640	50.0
Isopropyl butyrate	9.209	5.4	ug/L	141402	2	9.415	1318520	50.0