

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012125\
 Data File : VX044686.D
 Acq On : 21 Jan 2025 17:18
 Operator : JC/MD
 Sample : PB166134ZHE#11 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PB166134ZHE#11

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
 Title : VOC Analysis

Signal : TIC: VX044686.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	32	rBV	36335	50093	3.69%	0.504%
2	1.368	43	46	58	rBV	154340	198727	14.65%	2.001%
3	1.648	89	92	109	rVB	45436	99185	7.31%	0.999%
4	2.294	192	198	208	rBV	231880	369002	27.21%	3.716%
5	2.386	209	213	221	rVB	7530	14577	1.07%	0.147%
6	2.556	237	241	242	rBV3	393	506	0.04%	0.005%
7	2.624	250	252	253	rBV	535	360	0.03%	0.004%
8	2.672	258	260	264	rBV4	525	879	0.06%	0.009%
9	2.782	274	278	284	rVB5	1444	2635	0.19%	0.027%
10	2.941	296	304	313	rBV	10694	27696	2.04%	0.279%
11	3.075	325	326	327	rBV	776	406	0.03%	0.004%
12	3.166	338	341	342	rBV3	553	500	0.04%	0.005%
13	3.251	353	355	359	rVB4	565	615	0.05%	0.006%
14	3.337	367	369	371	rBV2	634	430	0.03%	0.004%
15	3.361	371	373	374	rVB	627	346	0.03%	0.003%
16	3.386	374	377	378	rBV3	402	448	0.03%	0.005%
17	3.434	378	385	392	rBV5	4455	10391	0.77%	0.105%
18	3.575	402	408	421	rVB2	10033	25650	1.89%	0.258%
19	3.660	421	422	424	rBV2	560	358	0.03%	0.004%
20	3.849	451	453	457	rBV2	585	559	0.04%	0.006%
21	3.904	459	462	468	rVB5	732	1508	0.11%	0.015%
22	3.959	468	471	472	rBV2	791	778	0.06%	0.008%
23	3.995	475	477	479	rBV2	386	343	0.03%	0.003%
24	4.129	496	499	501	rBV2	403	606	0.04%	0.006%
25	4.459	545	553	569	rBV	66555	224661	16.57%	2.263%
26	4.898	622	625	627	rVV3	549	499	0.04%	0.005%
27	4.965	633	636	637	rBV3	418	408	0.03%	0.004%
28	5.050	637	650	667	rVV	170307	537153	39.61%	5.410%
29	5.312	691	693	695	rBV2	657	620	0.05%	0.006%
30	5.361	699	701	702	rBV3	610	608	0.04%	0.006%
31	5.532	726	729	731	rBV4	688	717	0.05%	0.007%
32	5.684	752	754	757	rVB4	504	588	0.04%	0.006%
33	5.714	757	759	760	rBV2	617	409	0.03%	0.004%
34	5.745	762	764	767	rBV2	561	350	0.03%	0.004%
35	5.818	774	776	779	rBV4	431	455	0.03%	0.005%
36	5.855	779	782	783	rBV3	357	383	0.03%	0.004%

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37	5.873	783	785	787	rVB2	512	470	0.03%	0.005%
38	5.958	787	799	823	rBV2	448048	1356171	100.00%	13.658%
39	6.342	856	862	876	rVB3	8845	26286	1.94%	0.265%
40	6.751	920	929	954	rBV	268205	686314	50.61%	6.912%
41	7.300	1011	1019	1037	rBV	278400	624586	46.06%	6.290%
42	7.659	1073	1078	1083	rBV2	3073	6587	0.49%	0.066%
43	7.799	1095	1101	1119	rBV	110135	229346	16.91%	2.310%
44	8.171	1159	1162	1163	rVB2	380	381	0.03%	0.004%
45	8.232	1166	1172	1177	rBV7	579	1670	0.12%	0.017%
46	8.275	1177	1179	1180	rBV	559	434	0.03%	0.004%
47	8.318	1180	1186	1200	rBV	205110	357152	26.34%	3.597%
48	8.549	1218	1224	1233	rBV	27388	50718	3.74%	0.511%
49	8.641	1233	1239	1265	rVB	611934	1058953	78.08%	10.664%
50	8.946	1284	1289	1308	rBV2	164737	288913	21.30%	2.910%
51	9.244	1333	1338	1347	rBV	42667	65734	4.85%	0.662%
52	9.385	1356	1361	1372	rBV	282866	450602	33.23%	4.538%
53	9.482	1373	1377	1385	rVV	61003	87973	6.49%	0.886%
54	9.580	1389	1393	1405	rVV	36500	59519	4.39%	0.599%
55	9.702	1409	1413	1420	rVB4	3007	5860	0.43%	0.059%
56	9.909	1442	1447	1456	rBV	126360	182405	13.45%	1.837%
57	10.049	1465	1470	1489	rVB	527586	777579	57.34%	7.831%
58	10.287	1506	1509	1513	rBV4	1396	2074	0.15%	0.021%
59	10.378	1523	1524	1526	rBV	863	569	0.04%	0.006%
60	10.531	1543	1549	1553	rBV6	1258	2633	0.19%	0.027%
61	10.640	1561	1567	1579	rBV2	7956	15854	1.17%	0.160%
62	10.762	1586	1587	1590	rBV3	304	329	0.02%	0.003%
63	10.957	1617	1619	1621	rBV3	440	361	0.03%	0.004%
64	11.140	1646	1649	1652	rBV3	415	563	0.04%	0.006%
65	11.189	1652	1657	1669	rVV	451350	585227	43.15%	5.894%
66	11.445	1695	1699	1700	rBV2	415	563	0.04%	0.006%
67	11.707	1739	1742	1743	rBV3	435	536	0.04%	0.005%
68	11.732	1745	1746	1748	rVB	751	406	0.03%	0.004%
69	11.762	1748	1751	1756	rBV4	958	1275	0.09%	0.013%
70	11.805	1756	1758	1762	rBV3	608	593	0.04%	0.006%
71	11.860	1765	1767	1770	rVB3	531	534	0.04%	0.005%
72	11.890	1770	1772	1773	rBV	642	435	0.03%	0.004%
73	11.976	1781	1786	1788	rBV4	1014	1269	0.09%	0.013%
74	12.018	1788	1793	1806	rBV	499657	631234	46.55%	6.357%
75	12.177	1817	1819	1822	rBV3	429	346	0.03%	0.003%
76	12.317	1837	1842	1850	rBV	608982	779187	57.45%	7.847%

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Integration Parameters: LSCINT.P

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77	12.482	1867	1869	1870	rBV2	689	550	0.04%	0.006%
78	12.573	1883	1884	1886	rBV2	499	340	0.03%	0.003%
79	12.683	1901	1902	1906	rVB4	344	365	0.03%	0.004%
80	12.719	1906	1908	1909	rBV2	582	410	0.03%	0.004%
81	12.890	1933	1936	1939	rBV3	609	1146	0.08%	0.012%
82	13.000	1951	1954	1956	rVB	418	504	0.04%	0.005%
83	13.030	1956	1959	1960	rBV2	405	357	0.03%	0.004%
84	13.122	1971	1974	1977	rBV3	684	934	0.07%	0.009%
85	13.207	1987	1988	1993	rVB3	518	561	0.04%	0.006%
86	13.256	1993	1996	1997	rBV2	419	342	0.03%	0.003%
87	13.317	2004	2006	2008	rVV	425	437	0.03%	0.004%
88	13.372	2012	2015	2020	rVB3	558	861	0.06%	0.009%
89	13.439	2020	2026	2027	rBV4	510	857	0.06%	0.009%
90	13.664	2060	2063	2065	rVV3	495	435	0.03%	0.004%
91	14.243	2156	2158	2161	rBV3	484	644	0.05%	0.006%
92	14.518	2200	2203	2204	rBV2	580	493	0.04%	0.005%
93	14.688	2229	2231	2234	rBV3	506	635	0.05%	0.006%
94	14.768	2242	2244	2246	rBV2	636	651	0.05%	0.007%
95	14.884	2260	2263	2264	rBV2	453	567	0.04%	0.006%
96	14.975	2275	2278	2279	rBV3	599	617	0.05%	0.006%
97	15.377	2342	2344	2347	rBV3	577	518	0.04%	0.005%
98	15.804	2413	2414	2417	rBV4	706	439	0.03%	0.004%
99	16.395	2509	2511	2514	rBV2	775	1071	0.08%	0.011%
100	16.542	2533	2535	2538	rBV3	734	906	0.07%	0.009%

Sum of corrected areas: 9929730

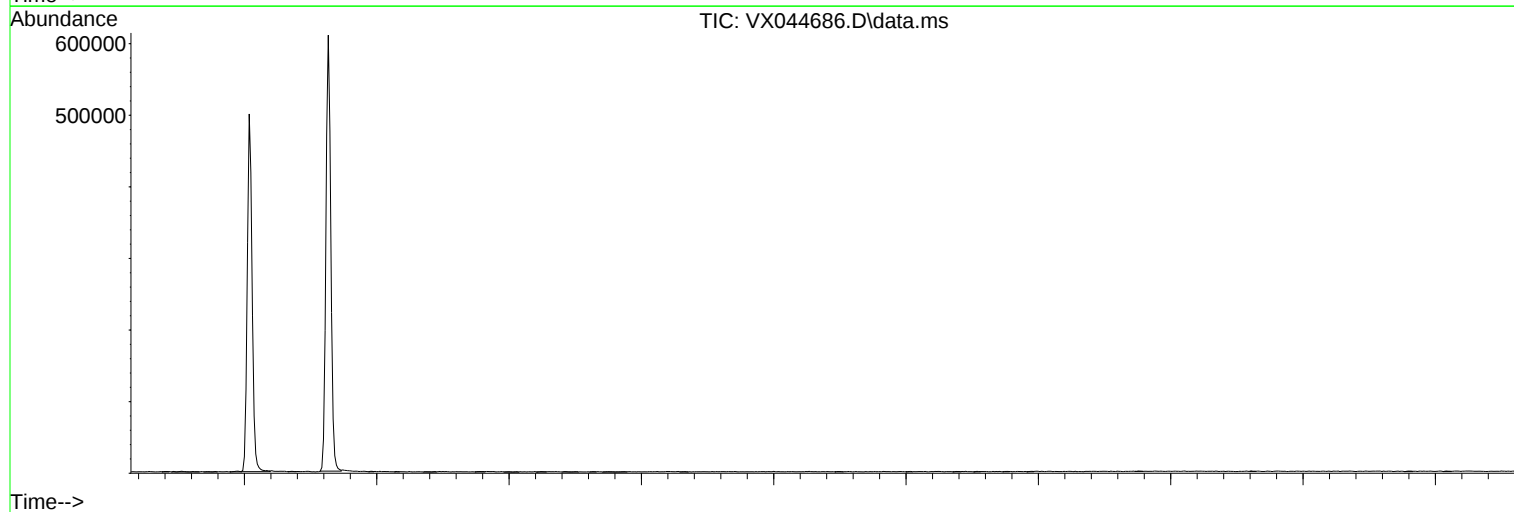
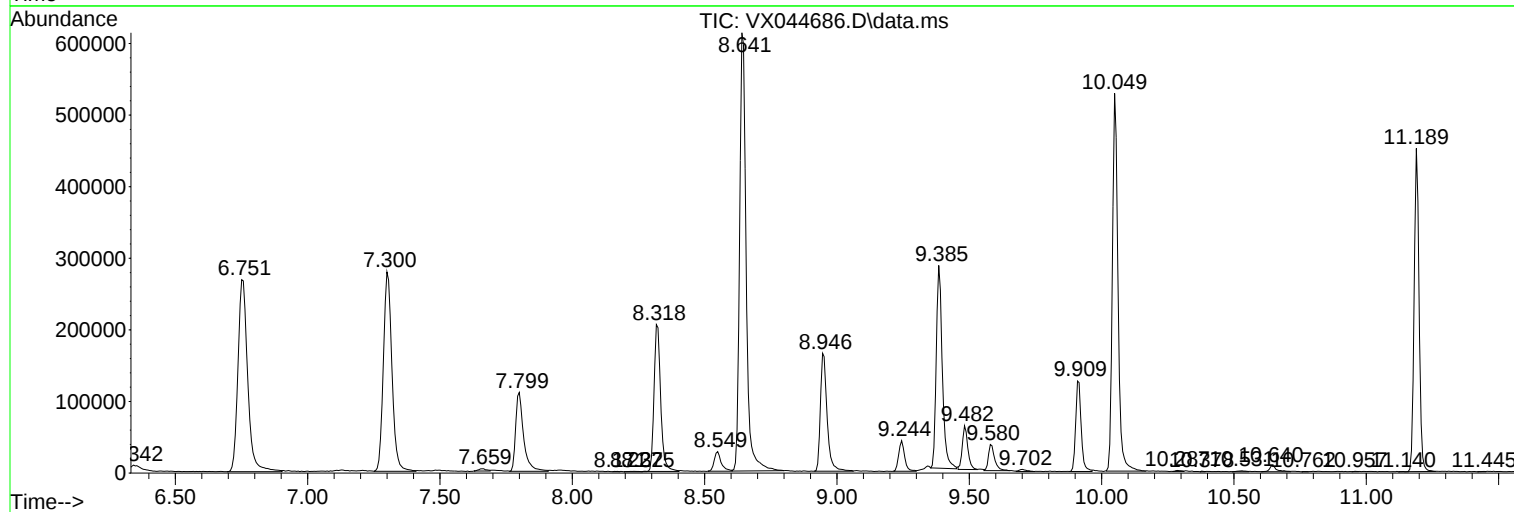
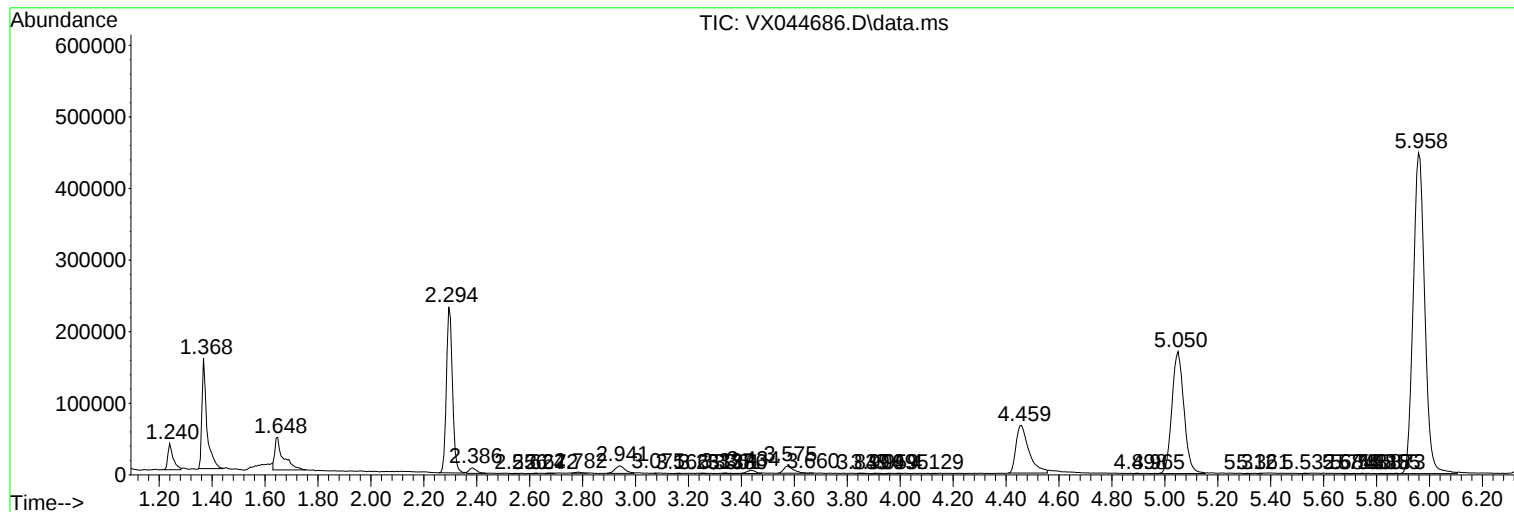
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Quant Title : VOC Analysis

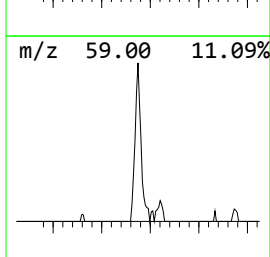
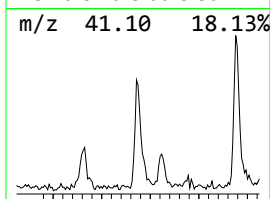
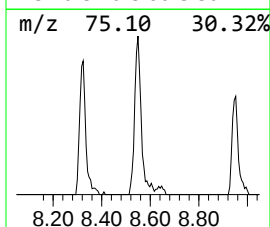
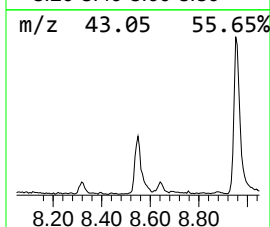
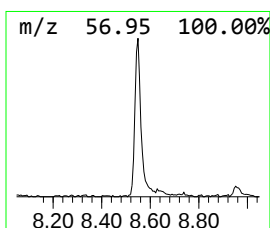
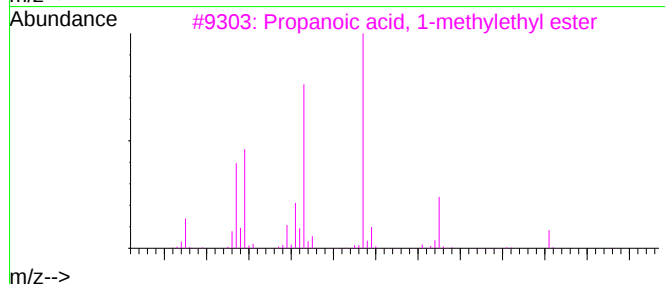
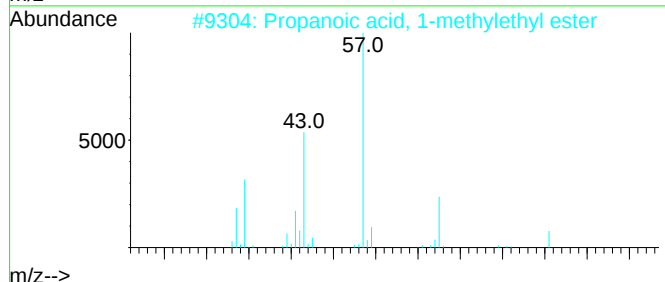
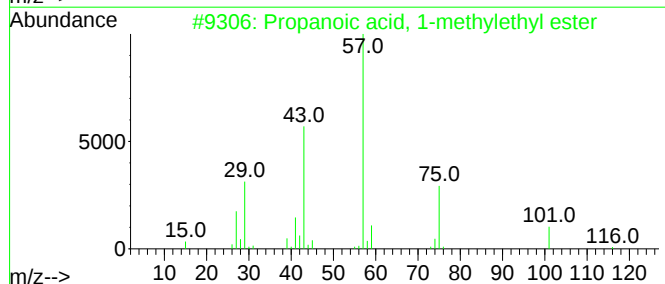
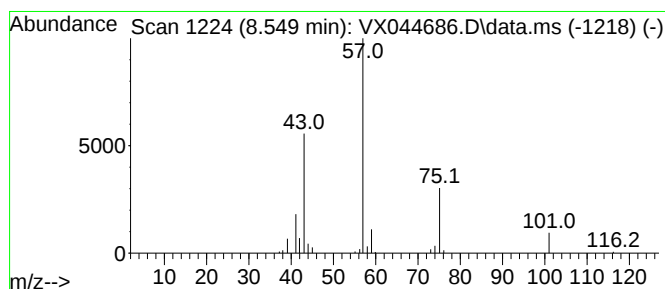
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	3.26 ug/L	50718	Chlorobenzene-d5	10.049

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	86
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50



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Quant Title : VOC Analysis

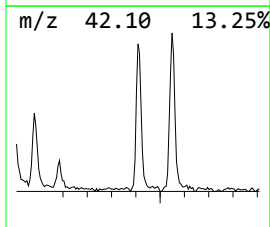
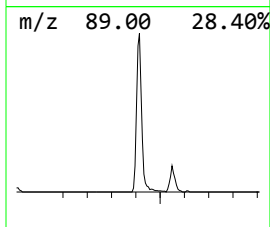
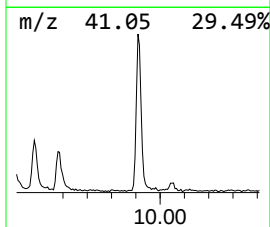
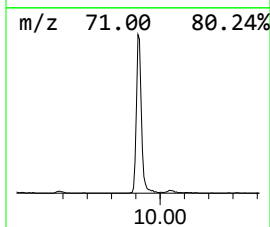
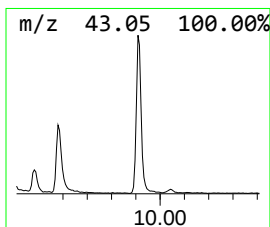
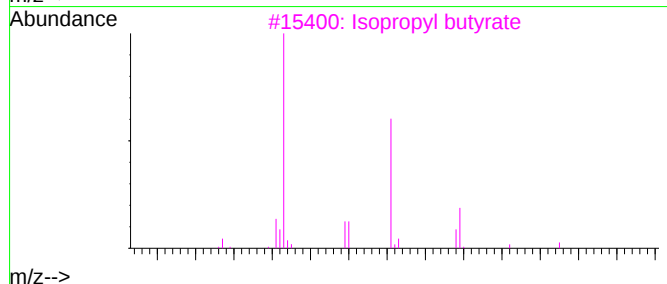
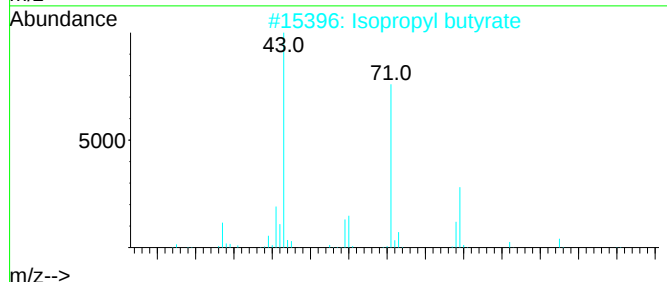
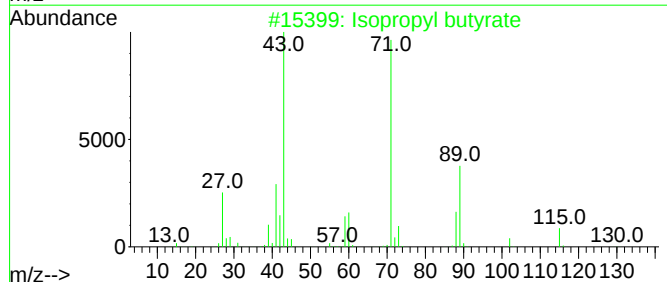
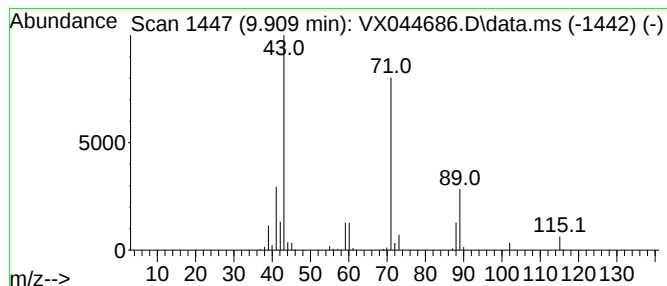
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.909	11.73 ug/L	182405	Chlorobenzene-d5	10.049

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-, 1-met...	130	C7H14O2	000617-50-5	72
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
Propanoic acid,...	8.549	3.3	ug/L	50718	2	10.049	777579	50.0
Isopropyl butyrate	9.909	11.7	ug/L	182405	2	10.049	777579	50.0