

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012125\
 Data File : VX044687.D
 Acq On : 21 Jan 2025 17:41
 Operator : JC/MD
 Sample : Q1130-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 JNLA7

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: VX044687.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	32	rBV	32510	45073	2.14%	0.322%
2	1.367	43	46	63	rVB	241569	317315	15.05%	2.269%
3	1.648	88	92	110	rVB	73918	141607	6.72%	1.013%
4	2.294	192	198	209	rBV	346153	559116	26.53%	3.998%
5	2.386	209	213	216	rBV	4848	7740	0.37%	0.055%
6	2.501	230	232	233	rBV	900	764	0.04%	0.005%
7	2.776	275	277	288	rVB6	1612	2875	0.14%	0.021%
8	2.867	290	292	293	rVB2	723	493	0.02%	0.004%
9	2.886	293	295	296	rBV2	532	487	0.02%	0.003%
10	2.940	297	304	315	rBV	9888	24004	1.14%	0.172%
11	3.081	323	327	330	rBV3	675	856	0.04%	0.006%
12	3.203	345	347	349	rBV2	497	573	0.03%	0.004%
13	3.434	379	385	391	rBV4	3411	7747	0.37%	0.055%
14	3.818	446	448	449	rBV	567	284	0.01%	0.002%
15	3.867	453	456	459	rBV4	511	848	0.04%	0.006%
16	4.056	484	487	488	rBV3	496	506	0.02%	0.004%
17	4.135	498	500	503	rBV3	616	670	0.03%	0.005%
18	4.312	526	529	530	rVB2	474	398	0.02%	0.003%
19	4.330	530	532	534	rBV3	278	320	0.02%	0.002%
20	4.452	543	552	580	rBV	109810	370542	17.58%	2.649%
21	4.946	631	633	636	rBV2	497	542	0.03%	0.004%
22	5.050	638	650	667	rVV	267008	828618	39.31%	5.925%
23	5.635	743	746	749	rBV3	665	855	0.04%	0.006%
24	5.739	762	763	768	rVB3	662	680	0.03%	0.005%
25	5.781	768	770	773	rBV3	341	462	0.02%	0.003%
26	5.830	775	778	780	rBV2	470	519	0.02%	0.004%
27	5.879	783	786	787	rBV2	523	601	0.03%	0.004%
28	5.958	787	799	821	rBV2	698134	2107770	100.00%	15.071%
29	6.348	855	863	871	rBV	7508	20868	0.99%	0.149%
30	6.586	899	902	903	rBV2	453	544	0.03%	0.004%
31	6.629	907	909	910	rBV	843	683	0.03%	0.005%
32	6.671	914	916	918	rBV2	461	373	0.02%	0.003%
33	6.751	920	929	956	rBV	351169	891584	42.30%	6.375%
34	7.104	983	987	988	rBV2	1779	2360	0.11%	0.017%
35	7.299	1011	1019	1038	rBV	436021	974608	46.24%	6.969%
36	7.659	1075	1078	1085	rBV2	2118	3763	0.18%	0.027%

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Integrator: RTE

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Max Peaks: 100

Peak Location: TOP

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Peak separation: 5

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

37	7.799	1096	1101	1121	rBV	46386	96736	4.59%	0.692%
38	8.025	1136	1138	1142	rBV4	671	920	0.04%	0.007%
39	8.183	1163	1164	1166	rBV2	450	261	0.01%	0.002%
40	8.220	1168	1170	1172	rBV3	363	248	0.01%	0.002%
41	8.317	1180	1186	1202	rBV	327501	559748	26.56%	4.002%
42	8.549	1216	1224	1231	rBV	20459	38925	1.85%	0.278%
43	8.641	1233	1239	1265	rVB	958125	1658258	78.67%	11.857%
44	8.945	1284	1289	1303	rBV	235151	362945	17.22%	2.595%
45	9.244	1333	1338	1346	rBV	30013	45331	2.15%	0.324%
46	9.323	1348	1351	1352	rVV	2067	2436	0.12%	0.017%
47	9.384	1356	1361	1374	rVV	444428	712730	33.81%	5.096%
48	9.488	1374	1378	1390	rVB	19409	35743	1.70%	0.256%
49	9.701	1409	1413	1417	rVB4	3481	4628	0.22%	0.033%
50	9.811	1429	1431	1436	rBV5	677	862	0.04%	0.006%
51	9.915	1443	1448	1456	rBV	50856	74120	3.52%	0.530%
52	10.049	1465	1470	1488	rBV	699438	1018960	48.34%	7.286%
53	10.195	1492	1494	1500	rVB4	1206	1545	0.07%	0.011%
54	10.494	1541	1543	1544	rBV2	344	329	0.02%	0.002%
55	10.713	1576	1579	1580	rBV3	564	535	0.03%	0.004%
56	10.787	1589	1591	1592	rBV2	380	251	0.01%	0.002%
57	10.805	1592	1594	1596	rVB2	705	570	0.03%	0.004%
58	10.872	1602	1605	1607	rBV3	468	611	0.03%	0.004%
59	10.915	1611	1612	1615	rVB3	786	625	0.03%	0.004%
60	10.951	1615	1618	1619	rBV3	662	820	0.04%	0.006%
61	11.079	1637	1639	1641	rBV3	516	624	0.03%	0.004%
62	11.189	1652	1657	1667	rBV	711163	914795	43.40%	6.541%
63	11.396	1689	1691	1693	rBV3	569	617	0.03%	0.004%
64	11.439	1695	1698	1699	rBV2	461	614	0.03%	0.004%
65	11.506	1707	1709	1712	rVB3	523	597	0.03%	0.004%
66	11.561	1715	1718	1720	rVB3	568	511	0.02%	0.004%
67	11.707	1739	1742	1747	rVB6	1616	1635	0.08%	0.012%
68	11.805	1756	1758	1759	rVB	736	413	0.02%	0.003%
69	11.823	1759	1761	1762	rBV2	490	358	0.02%	0.003%
70	11.969	1783	1785	1788	rVB3	1074	1217	0.06%	0.009%
71	12.018	1788	1793	1804	rBV	679525	852557	40.45%	6.096%
72	12.317	1837	1842	1855	rBV	999915	1260186	59.79%	9.011%
73	12.719	1906	1908	1909	rVB2	494	245	0.01%	0.002%
74	12.847	1927	1929	1930	rBV	555	410	0.02%	0.003%
75	12.865	1930	1932	1934	rBV2	500	502	0.02%	0.004%
76	12.926	1940	1942	1946	rVB2	516	690	0.03%	0.005%

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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_X\Method\SFAMXML012125WMA.M
 Title : VOC Analysis

77	13.000	1952	1954	1962	rVB4	554	747	0.04%	0.005%
78	13.079	1965	1967	1968	rVB2	500	311	0.01%	0.002%
79	13.091	1968	1969	1971	rBV2	647	538	0.03%	0.004%
80	13.176	1980	1983	1984	rBV3	392	526	0.02%	0.004%
81	13.298	2001	2003	2007	rBV3	438	728	0.03%	0.005%
82	13.353	2010	2012	2014	rVV3	479	361	0.02%	0.003%
83	13.371	2014	2015	2017	rVV2	431	242	0.01%	0.002%
84	13.579	2046	2049	2050	rBV2	532	534	0.03%	0.004%
85	13.603	2050	2053	2055	rBV2	719	954	0.05%	0.007%
86	13.786	2081	2083	2087	rBV4	600	775	0.04%	0.006%
87	13.847	2092	2093	2097	rVB3	514	542	0.03%	0.004%
88	13.884	2097	2099	2102	rBV4	614	709	0.03%	0.005%
89	13.969	2110	2113	2114	rBV3	639	675	0.03%	0.005%
90	14.073	2128	2130	2131	rBV	625	477	0.02%	0.003%
91	14.127	2136	2139	2140	rBV3	692	721	0.03%	0.005%
92	14.170	2145	2146	2147	rBV	575	281	0.01%	0.002%
93	14.188	2147	2149	2151	rBV3	447	415	0.02%	0.003%
94	14.347	2172	2175	2177	rBV4	526	717	0.03%	0.005%
95	14.396	2181	2183	2184	rBV2	602	369	0.02%	0.003%
96	14.444	2189	2191	2196	rVB4	1314	1787	0.08%	0.013%
97	14.481	2196	2197	2198	rBV	695	266	0.01%	0.002%
98	14.585	2212	2214	2218	rBV3	539	691	0.03%	0.005%
99	14.798	2248	2249	2254	rBV3	572	574	0.03%	0.004%
100	16.651	2552	2553	2554	rVB	772	282	0.01%	0.002%

Sum of corrected areas: 13985378

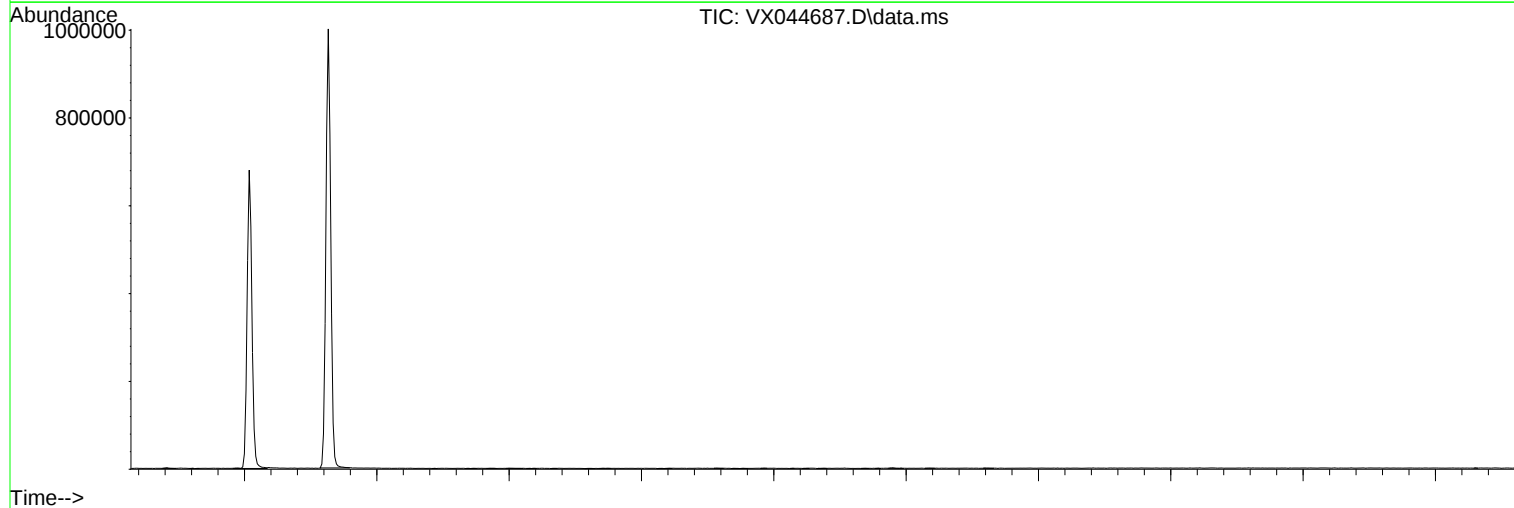
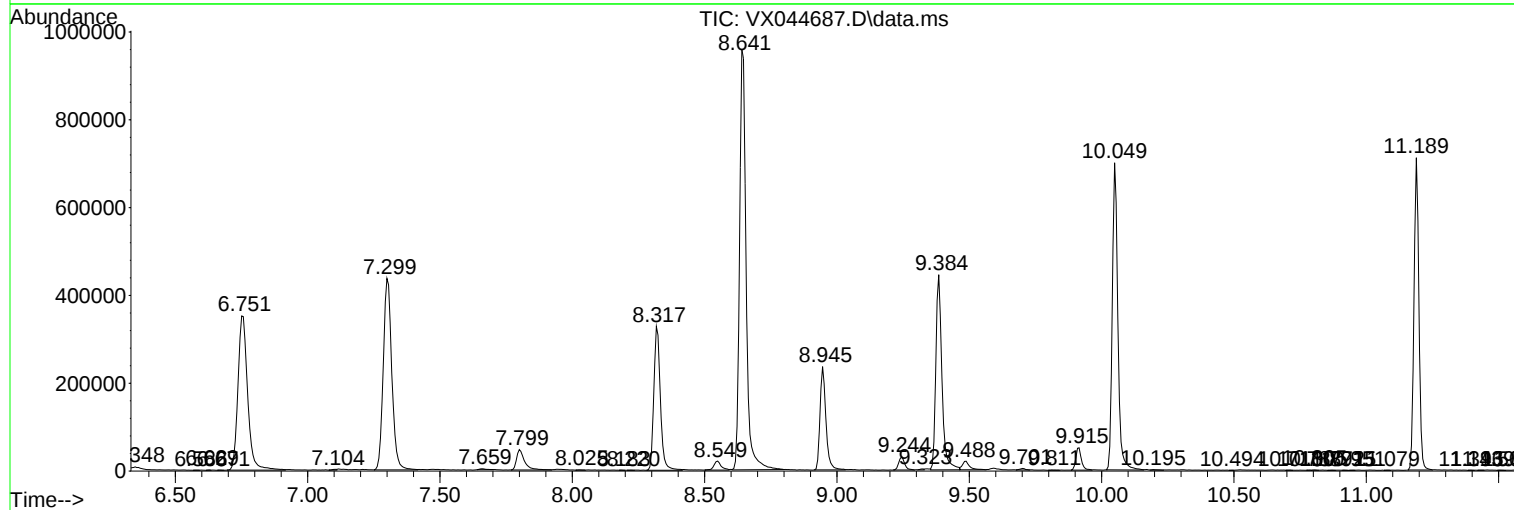
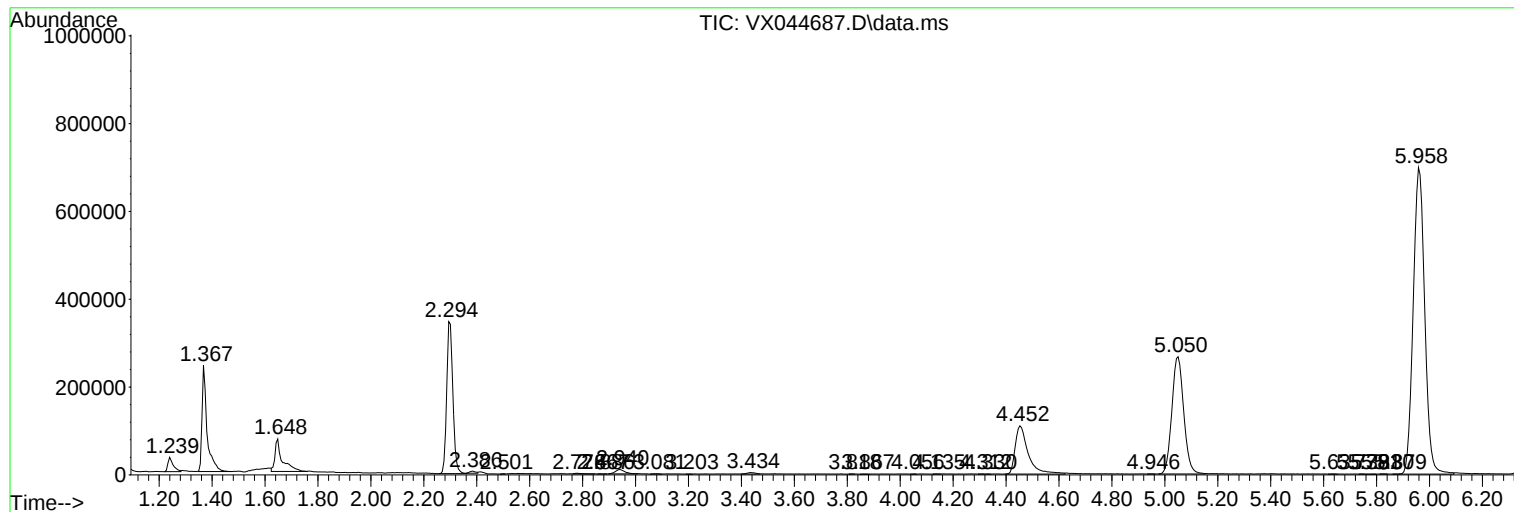
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012125WMA.M
Quant Title : VOC Analysis

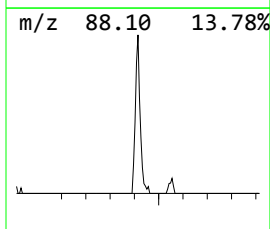
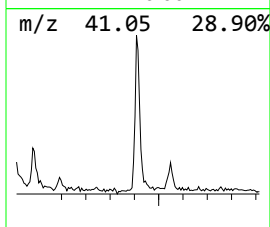
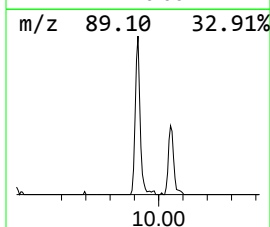
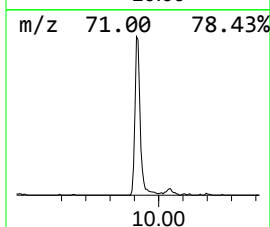
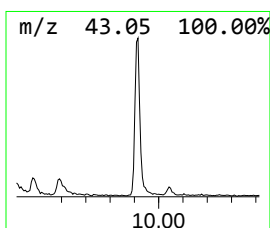
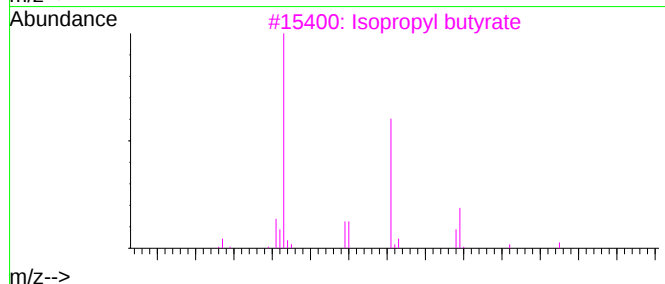
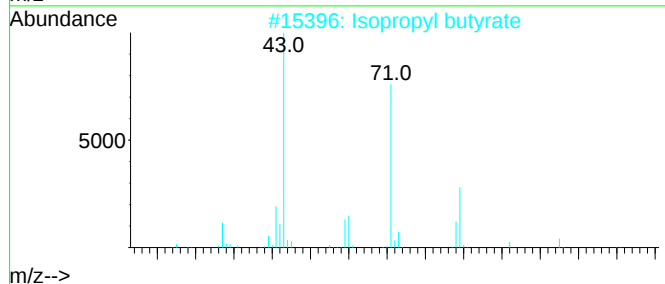
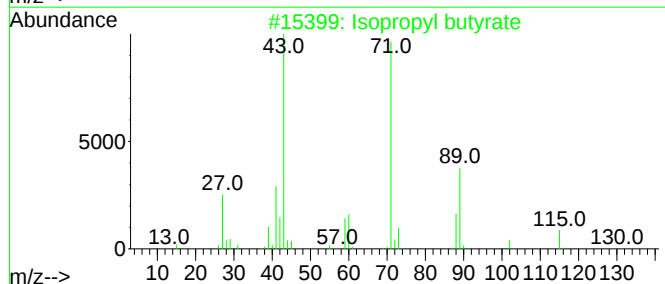
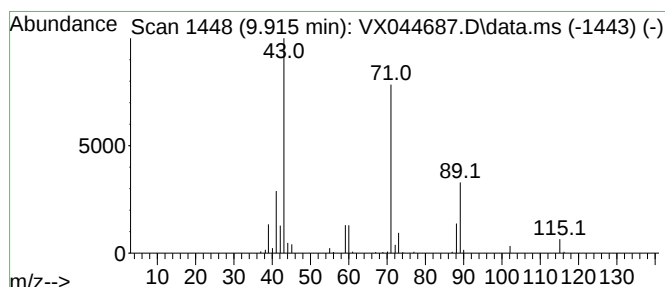
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	3.64 ug/L	74120	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	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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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl butyrate	9.915	3.6	ug/L	74120	2	10.049	1018960	50.0