

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012825\
 Data File : VX044749.D
 Acq On : 28 Jan 2025 17:07
 Operator : JC/MD
 Sample : Q1162-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E2946

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\SFAMXML012825WMA.M
 Title : VOC Analysis

Signal : TIC: VX044749.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	34	rBV	15974	25860	2.31%	0.304%
2	1.368	42	46	59	rBV	144472	161907	14.46%	1.903%
3	1.648	88	92	101	rVB	78120	103239	9.22%	1.214%
4	2.300	193	199	208	rVV	240817	393148	35.11%	4.622%
5	2.380	209	212	222	rVB	7738	13904	1.24%	0.163%
6	2.557	236	241	249	rVB4	2036	5084	0.45%	0.060%
7	2.843	286	288	292	rVB2	513	479	0.04%	0.006%
8	2.880	292	294	295	rBV2	378	322	0.03%	0.004%
9	2.935	295	303	315	rVV	14999	38661	3.45%	0.454%
10	3.270	356	358	360	rVB2	353	358	0.03%	0.004%
11	3.300	360	363	364	rBV	486	513	0.05%	0.006%
12	3.367	373	374	379	rVB	430	539	0.05%	0.006%
13	3.428	382	384	385	rBV	735	634	0.06%	0.007%
14	3.764	438	439	442	rBV	453	437	0.04%	0.005%
15	3.855	452	454	455	rBV	415	318	0.03%	0.004%
16	3.904	459	462	463	rBV2	612	500	0.04%	0.006%
17	4.026	481	482	485	rBV3	523	457	0.04%	0.005%
18	4.148	501	502	506	rBV3	422	535	0.05%	0.006%
19	4.282	522	524	527	rBV3	355	388	0.03%	0.005%
20	4.459	545	553	569	rBV	69636	215828	19.27%	2.537%
21	5.050	638	650	667	rBV	134955	431608	38.54%	5.074%
22	5.373	701	703	704	rBV	527	434	0.04%	0.005%
23	5.458	714	717	718	rVB3	423	369	0.03%	0.004%
24	5.556	730	733	736	rVV2	559	753	0.07%	0.009%
25	5.690	750	755	756	rBV	383	440	0.04%	0.005%
26	5.800	769	773	776	rBV	282	503	0.04%	0.006%
27	5.964	787	800	825	rBV2	373604	1119834	100.00%	13.164%
28	6.349	858	863	874	rVB2	3896	11477	1.02%	0.135%
29	6.568	896	899	901	rBV2	246	357	0.03%	0.004%
30	6.757	921	930	954	rBV	301422	743364	66.38%	8.739%
31	6.964	962	964	967	rBV3	553	611	0.05%	0.007%
32	7.007	969	971	973	rBV3	359	379	0.03%	0.004%
33	7.123	984	990	995	rVB8	1435	2688	0.24%	0.032%
34	7.165	995	997	1001	rVB3	500	597	0.05%	0.007%
35	7.208	1001	1004	1007	rBV	695	744	0.07%	0.009%
36	7.239	1007	1009	1011	rBV	458	449	0.04%	0.005%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
 Title : VOC Analysis

37	7.306	1011	1020	1037	rBV	225766	509360	45.49%	5.988%
38	7.659	1072	1078	1088	rBV	3109	8067	0.72%	0.095%
39	7.812	1098	1103	1112	rBV	8850	18410	1.64%	0.216%
40	7.952	1124	1126	1128	rBV3	652	568	0.05%	0.007%

41	8.324	1180	1187	1205	rBV	159983	281558	25.14%	3.310%
42	8.549	1217	1224	1233	rBV	12811	26280	2.35%	0.309%
43	8.647	1233	1240	1260	rVV	524969	888958	79.38%	10.450%
44	8.946	1284	1289	1305	rBV	113407	176116	15.73%	2.070%
45	9.208	1329	1332	1333	rVB	523	484	0.04%	0.006%

46	9.244	1333	1338	1346	rBV	20564	32619	2.91%	0.383%
47	9.324	1347	1351	1356	rBV4	1565	3367	0.30%	0.040%
48	9.385	1356	1361	1375	rBV	275293	427296	38.16%	5.023%
49	9.696	1409	1412	1416	rBV3	2408	2939	0.26%	0.035%
50	9.775	1422	1425	1427	rBV2	504	687	0.06%	0.008%

51	9.848	1432	1437	1438	rBV2	429	520	0.05%	0.006%
52	9.915	1441	1448	1457	rBV	39180	54915	4.90%	0.646%
53	10.049	1465	1470	1490	rBV	590893	864975	77.24%	10.168%
54	10.427	1530	1532	1536	rBV2	402	518	0.05%	0.006%
55	10.647	1564	1568	1569	rBV3	620	732	0.07%	0.009%

56	10.799	1590	1593	1594	rVV2	530	446	0.04%	0.005%
57	10.817	1594	1596	1598	rVB	537	371	0.03%	0.004%
58	10.964	1616	1620	1623	rBV4	612	653	0.06%	0.008%
59	11.189	1652	1657	1670	rVB	391316	505613	45.15%	5.944%
60	11.366	1685	1686	1690	rVB	422	375	0.03%	0.004%

61	11.403	1690	1692	1694	rBV	366	333	0.03%	0.004%
62	11.457	1698	1701	1703	rVV3	637	657	0.06%	0.008%
63	11.561	1716	1718	1721	rVV2	293	337	0.03%	0.004%
64	11.652	1729	1733	1736	rBV2	389	613	0.05%	0.007%
65	11.768	1748	1752	1756	rVB2	830	994	0.09%	0.012%

66	11.896	1772	1773	1778	rVB2	490	466	0.04%	0.005%
67	11.969	1782	1785	1788	rBV3	637	653	0.06%	0.008%
68	12.018	1788	1793	1808	rBV	569486	726656	64.89%	8.542%
69	12.226	1823	1827	1830	rBV5	1489	2296	0.21%	0.027%
70	12.317	1837	1842	1854	rBV	540636	667488	59.61%	7.847%

71	12.549	1875	1880	1882	rBV3	267	525	0.05%	0.006%
72	12.701	1904	1905	1908	rBV2	450	470	0.04%	0.006%
73	12.762	1912	1915	1919	rVB4	1173	1570	0.14%	0.018%
74	12.793	1919	1920	1922	rBV2	510	485	0.04%	0.006%
75	12.884	1932	1935	1938	rVB2	669	691	0.06%	0.008%

76	13.164	1975	1981	1982	rBV2	261	451	0.04%	0.005%
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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
 Title : VOC Analysis

77	13.238	1990	1993	1998	rVB2	546	941	0.08%	0.011%
78	13.494	2034	2035	2038	rVV2	377	375	0.03%	0.004%
79	13.561	2044	2046	2047	rBV	575	538	0.05%	0.006%
80	13.591	2049	2051	2058	rVB3	814	1373	0.12%	0.016%
81	13.676	2060	2065	2067	rBV2	535	903	0.08%	0.011%
82	13.750	2074	2077	2078	rBV2	265	347	0.03%	0.004%
83	13.780	2080	2082	2089	rVV5	1302	2111	0.19%	0.025%
84	13.890	2096	2100	2104	rBV4	564	841	0.08%	0.010%
85	13.951	2108	2110	2112	rVV2	373	339	0.03%	0.004%
86	14.030	2120	2123	2125	rBV3	666	997	0.09%	0.012%
87	14.128	2136	2139	2143	rVB2	1799	2023	0.18%	0.024%
88	14.219	2152	2154	2157	rBV2	304	495	0.04%	0.006%
89	14.378	2178	2180	2182	rVB2	565	396	0.04%	0.005%
90	14.506	2197	2201	2202	rBV2	300	321	0.03%	0.004%
91	14.658	2221	2226	2231	rVB4	727	1299	0.12%	0.015%
92	14.780	2243	2246	2253	rVB4	836	1513	0.14%	0.018%
93	14.963	2275	2276	2278	rVB	633	356	0.03%	0.004%
94	15.115	2296	2301	2302	rBV3	387	607	0.05%	0.007%
95	15.195	2312	2314	2316	rBV2	503	490	0.04%	0.006%
96	15.457	2353	2357	2359	rBV	474	625	0.06%	0.007%
97	16.005	2445	2447	2449	rBV2	572	408	0.04%	0.005%
98	16.298	2494	2495	2497	rBV2	565	349	0.03%	0.004%
99	16.316	2497	2498	2502	rVB3	610	434	0.04%	0.005%
100	16.426	2514	2516	2519	rBV2	494	410	0.04%	0.005%

Sum of corrected areas: 8506721

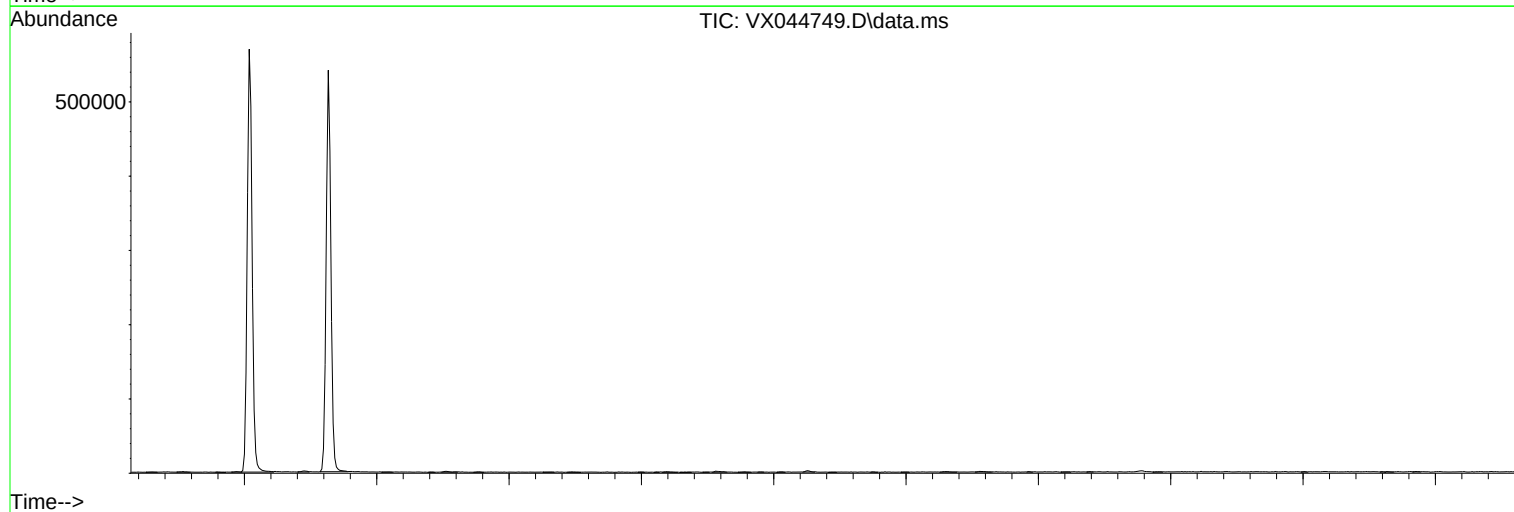
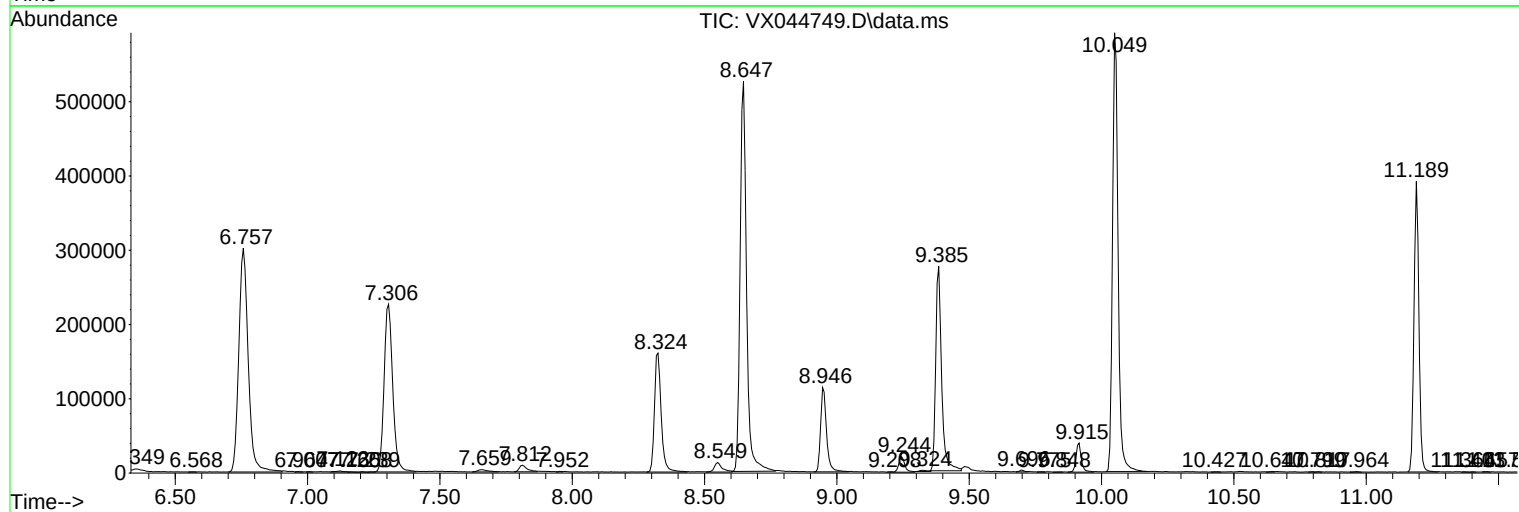
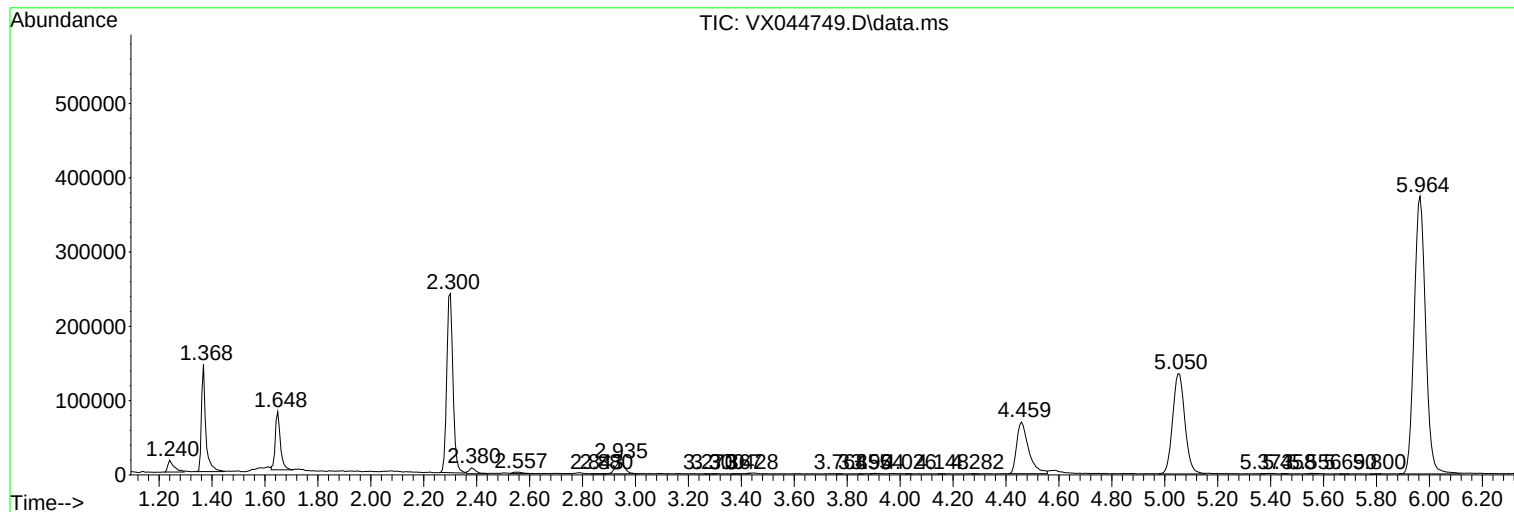
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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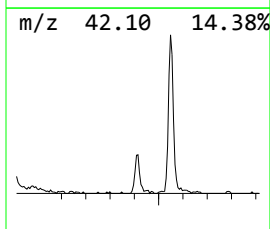
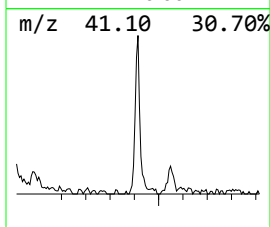
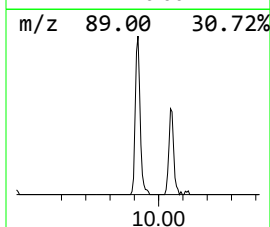
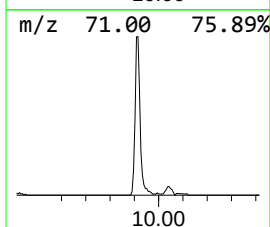
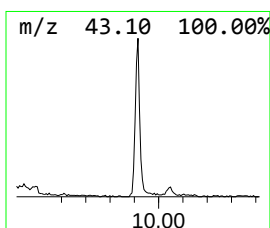
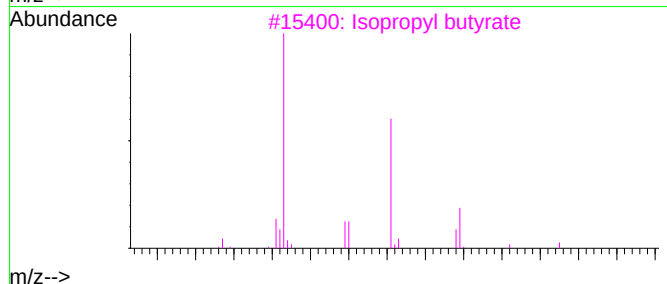
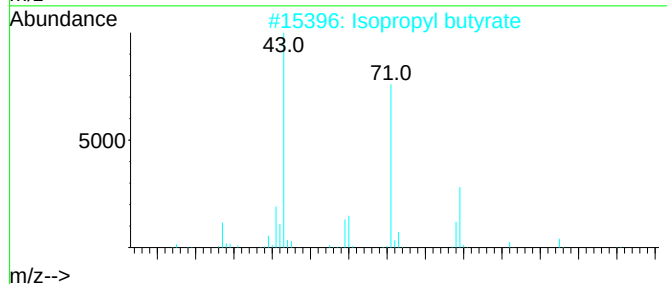
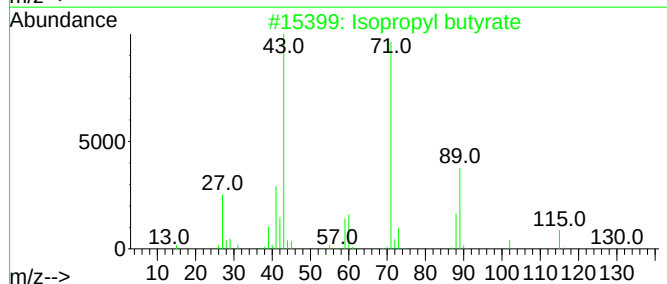
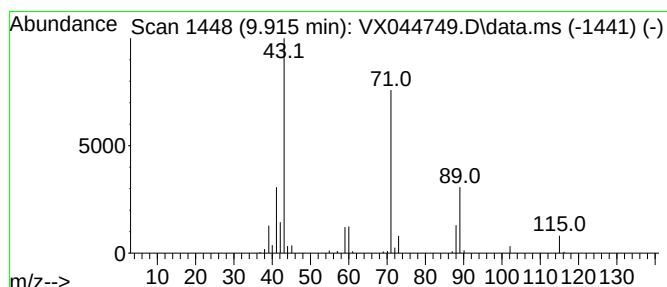
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	3.17 ug/L	54915	Chlorobenzene-d5	10.049

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	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl butyrate	9.915	3.2	ug/L	54915	2	10.049	864975	50.0