

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
 Data File : VX044521.D
 Acq On : 27 Dec 2024 15:22
 Operator : JC/MD
 Sample : P5326-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YE680

Integration Parameters: LSCINT.P

Integrator: RTE

Smothing : 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\SFAMXML120524WMA.M
 Title : VOC Analysis

Signal : TIC: VX044521.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	23	25	26	rBV	3032	2292	0.23%	0.030%
2	1.368	42	46	57	rBV	127636	156747	15.55%	2.083%
3	1.642	88	91	111	rVB	109283	173073	17.17%	2.300%
4	2.294	192	198	208	rBV	211375	334334	33.16%	4.443%
5	2.447	221	223	226	rVB2	544	541	0.05%	0.007%
6	2.550	238	240	241	rBV2	576	459	0.05%	0.006%
7	2.709	264	266	271	rVB3	1089	1513	0.15%	0.020%
8	2.782	274	278	286	rVB6	2015	3795	0.38%	0.050%
9	2.941	299	304	310	rVB	7371	15065	1.49%	0.200%
10	3.081	323	327	329	rBV4	1556	1897	0.19%	0.025%
11	3.422	380	383	384	rBV2	2410	2493	0.25%	0.033%
12	3.593	410	411	419	rVB5	880	1545	0.15%	0.021%
13	3.727	432	433	436	rVB2	520	425	0.04%	0.006%
14	3.794	442	444	447	rBV3	446	436	0.04%	0.006%
15	3.934	463	467	468	rVB2	610	430	0.04%	0.006%
16	3.965	468	472	473	rBV3	594	836	0.08%	0.011%
17	4.050	483	486	487	rBV2	402	434	0.04%	0.006%
18	4.465	543	554	567	rBV	57718	181761	18.03%	2.415%
19	4.806	608	610	611	rBV2	591	504	0.05%	0.007%
20	4.904	623	626	632	rVB4	857	1350	0.13%	0.018%
21	5.044	638	649	664	rBV2	133457	421741	41.83%	5.604%
22	5.294	686	690	693	rVB3	580	1000	0.10%	0.013%
23	5.446	712	715	717	rBV3	676	842	0.08%	0.011%
24	5.525	726	728	730	rBV2	634	728	0.07%	0.010%
25	5.641	745	747	749	rBV3	568	700	0.07%	0.009%
26	5.964	786	800	816	rBV2	333373	1008210	100.00%	13.397%
27	6.208	839	840	844	rVB3	722	655	0.06%	0.009%
28	6.348	856	863	871	rBV3	5454	14887	1.48%	0.198%
29	6.483	883	885	890	rVB3	697	908	0.09%	0.012%
30	6.519	890	891	894	rBV3	576	524	0.05%	0.007%
31	6.562	897	898	903	rVV3	593	656	0.07%	0.009%
32	6.684	917	918	921	rBV	954	676	0.07%	0.009%
33	6.757	921	930	947	rVV	207931	506098	50.20%	6.725%
34	6.964	961	964	965	rBV	595	444	0.04%	0.006%
35	7.123	983	990	999	rBV6	5812	14183	1.41%	0.188%
36	7.306	1010	1020	1029	rBV	203335	453372	44.97%	6.024%

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 Title : VOC Analysis

37	7.537	1055	1058	1060	rVB2	673	720	0.07%	0.010%
38	7.635	1070	1074	1075	rBV3	640	877	0.09%	0.012%
39	7.665	1075	1079	1082	rVV3	1550	2404	0.24%	0.032%
40	7.799	1094	1101	1114	rBV	65695	126532	12.55%	1.681%
41	7.940	1122	1124	1127	rBV2	696	723	0.07%	0.010%
42	8.208	1164	1168	1169	rBV2	394	485	0.05%	0.006%
43	8.324	1181	1187	1199	rBV	122104	206890	20.52%	2.749%
44	8.549	1218	1224	1233	rBV	14416	29590	2.93%	0.393%
45	8.647	1233	1240	1249	rBV	480305	762143	75.59%	10.127%
46	8.952	1285	1290	1300	rBV2	93203	158097	15.68%	2.101%
47	9.159	1320	1324	1328	rVB4	1342	2366	0.23%	0.031%
48	9.244	1332	1338	1347	rBV	19828	34200	3.39%	0.454%
49	9.348	1347	1355	1356	rBV4	3077	5391	0.53%	0.072%
50	9.384	1356	1361	1374	rVV	263410	401067	39.78%	5.329%
51	9.482	1374	1377	1384	rVB	26989	41083	4.07%	0.546%
52	9.586	1390	1394	1406	rVV	15371	26583	2.64%	0.353%
53	9.695	1410	1412	1417	rVB2	1029	1318	0.13%	0.018%
54	9.915	1443	1448	1456	rVV	52933	74304	7.37%	0.987%
55	10.000	1460	1462	1465	rVV4	510	642	0.06%	0.009%
56	10.049	1465	1470	1486	rVB	406985	590891	58.61%	7.852%
57	10.201	1491	1495	1498	rVB2	2413	3316	0.33%	0.044%
58	10.305	1505	1512	1520	rBV7	2271	5215	0.52%	0.069%
59	10.360	1520	1521	1524	rVB3	613	511	0.05%	0.007%
60	10.421	1527	1531	1532	rBV2	375	467	0.05%	0.006%
61	10.653	1562	1569	1580	rBV6	4495	11601	1.15%	0.154%
62	10.799	1592	1593	1598	rVB3	700	865	0.09%	0.011%
63	10.902	1608	1610	1613	rVB3	514	573	0.06%	0.008%
64	10.963	1616	1620	1625	rVV3	2434	3794	0.38%	0.050%
65	11.055	1632	1635	1636	rBV	639	527	0.05%	0.007%
66	11.091	1636	1641	1643	rVB3	451	743	0.07%	0.010%
67	11.189	1651	1657	1664	rBV	347740	457307	45.36%	6.077%
68	11.457	1696	1701	1707	rBV4	2346	3240	0.32%	0.043%
69	11.756	1747	1750	1755	rBV2	1993	3001	0.30%	0.040%
70	11.975	1783	1786	1788	rBV3	2073	2547	0.25%	0.034%
71	12.018	1788	1793	1803	rVV	429743	555206	55.07%	7.377%
72	12.256	1831	1832	1836	rBV	727	619	0.06%	0.008%
73	12.317	1837	1842	1857	rVV	535203	677091	67.16%	8.997%
74	12.591	1883	1887	1888	rBV	353	458	0.05%	0.006%
75	12.670	1899	1900	1903	rVV2	542	515	0.05%	0.007%
76	12.719	1905	1908	1909	rBV2	639	476	0.05%	0.006%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
 Title : VOC Analysis

77	12.762	1911	1915	1920	rVB4	1929	3459	0.34%	0.046%
78	12.847	1926	1929	1930	rBV2	553	424	0.04%	0.006%
79	12.866	1930	1932	1935	rBV	382	431	0.04%	0.006%
80	13.116	1971	1973	1977	rBV4	1024	1351	0.13%	0.018%
81	13.250	1993	1995	1996	rBV2	445	432	0.04%	0.006%
82	13.439	2024	2026	2032	rBV2	691	1016	0.10%	0.014%
83	13.530	2039	2041	2044	rVB3	678	630	0.06%	0.008%
84	13.567	2044	2047	2049	rBV	490	657	0.07%	0.009%
85	13.597	2049	2052	2056	rVB3	1134	1278	0.13%	0.017%
86	13.786	2079	2083	2088	rVV2	1614	2493	0.25%	0.033%
87	13.829	2088	2090	2093	rVB3	609	532	0.05%	0.007%
88	13.902	2100	2102	2106	rVB2	461	634	0.06%	0.008%
89	13.939	2106	2108	2110	rBV2	348	446	0.04%	0.006%
90	13.963	2110	2112	2118	rVB5	1094	1683	0.17%	0.022%
91	14.134	2133	2140	2143	rBV	3620	4970	0.49%	0.066%
92	14.365	2177	2178	2181	rVB3	553	473	0.05%	0.006%
93	14.414	2181	2186	2191	rBV3	829	1227	0.12%	0.016%
94	14.603	2214	2217	2219	rVB3	598	668	0.07%	0.009%
95	14.725	2236	2237	2241	rVB3	492	508	0.05%	0.007%
96	14.829	2251	2254	2256	rBV2	714	483	0.05%	0.006%
97	15.188	2311	2313	2314	rVV	659	436	0.04%	0.006%
98	15.225	2317	2319	2321	rBV3	613	516	0.05%	0.007%
99	15.816	2414	2416	2418	rBV2	657	479	0.05%	0.006%
100	16.298	2493	2495	2496	rBV	716	553	0.05%	0.007%

Sum of corrected areas: 7525711

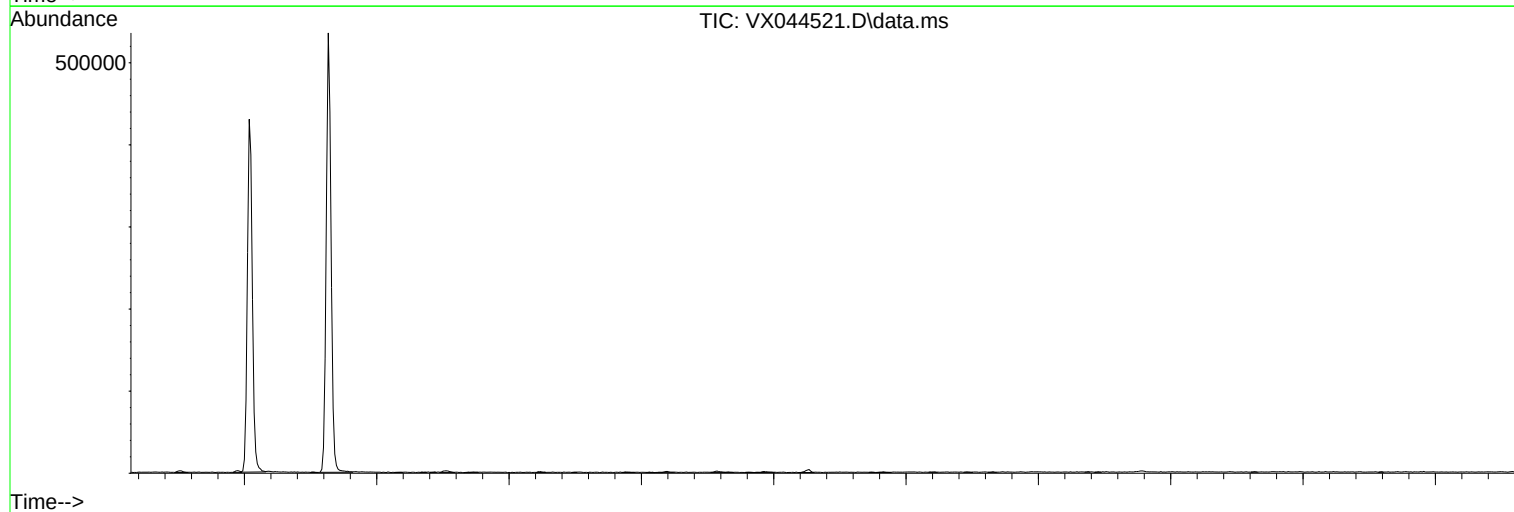
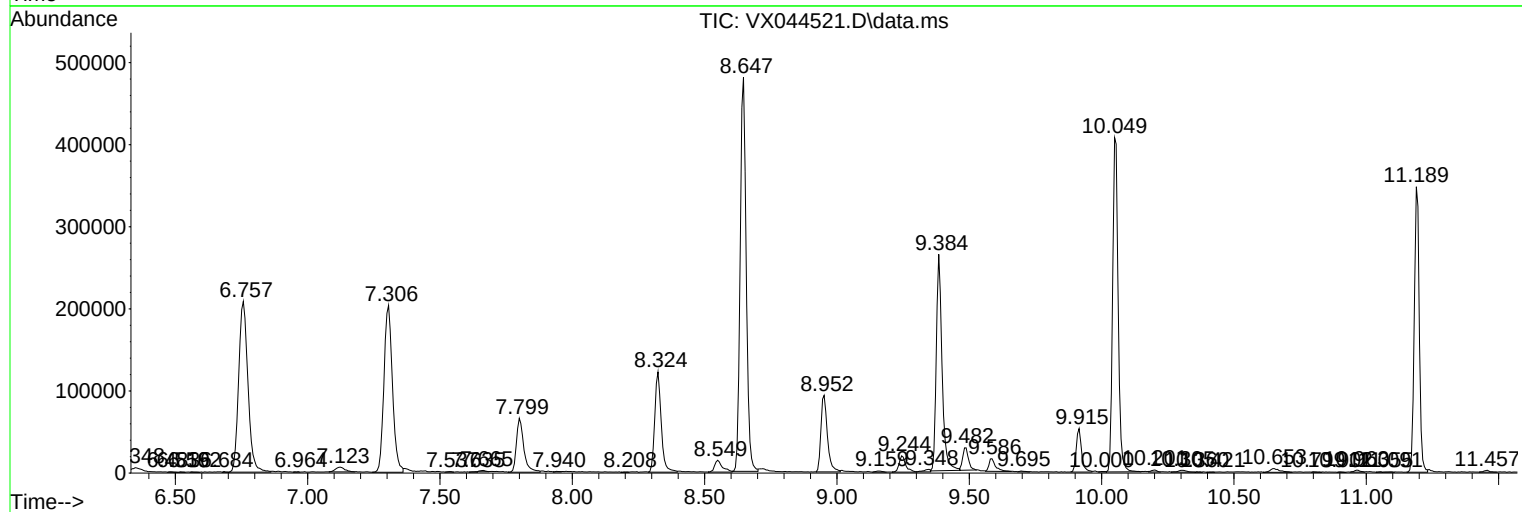
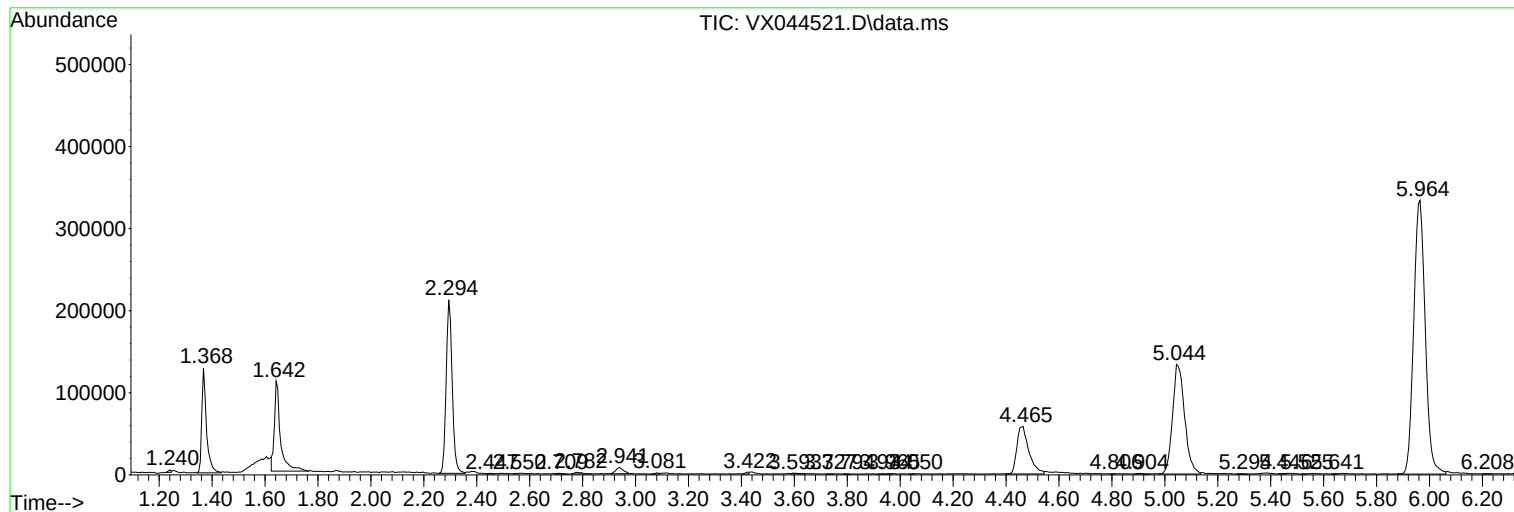
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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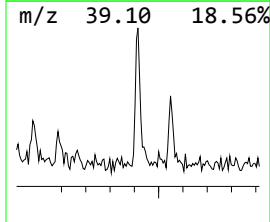
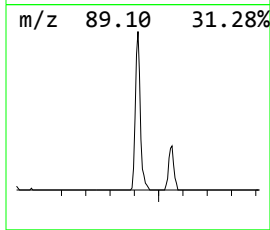
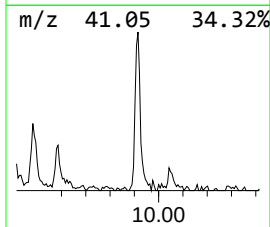
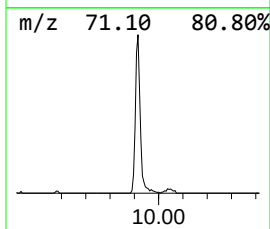
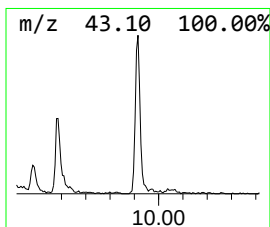
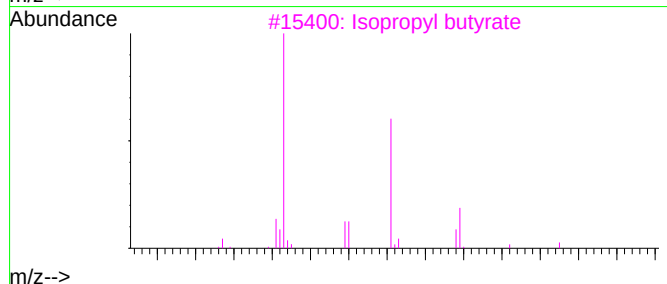
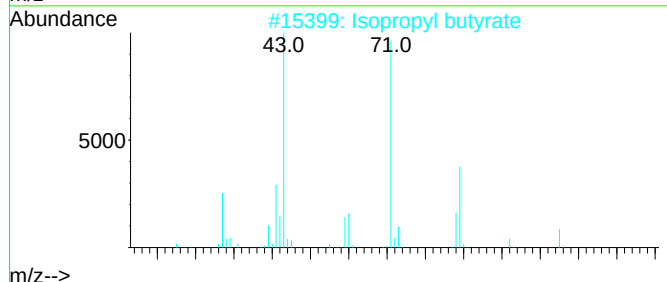
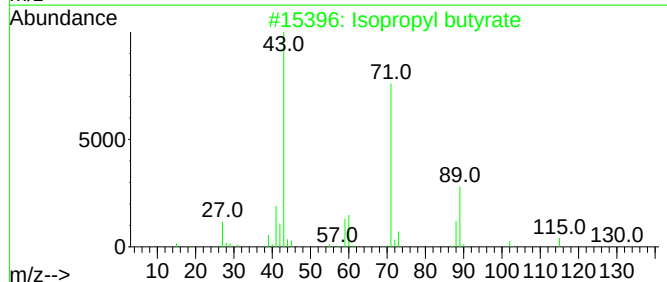
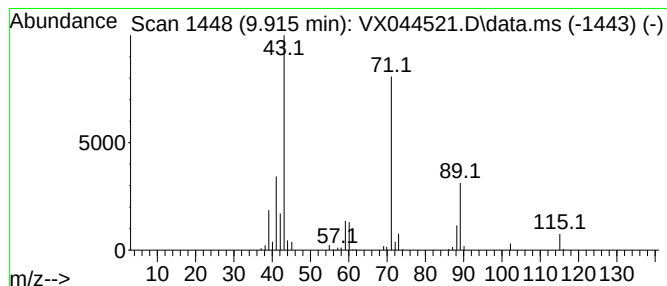
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	6.29 ug/L	74304	Chlorobenzene-d5	10.055

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	83
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	83
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl butyrate	9.915	6.3	ug/L	74304	2	10.055	590891	50.0