

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044344.D
 Acq On : 17 Dec 2024 12:22
 Operator : JC/MD
 Sample : P5235-03 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AT1

Integration Parameters: LSCINT.P

Integrator: RTE

Smoother: 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: VX044344.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	27	rBV2	3480	3333	0.33%	0.043%
2	1.368	42	46	56	rVB	117555	131814	13.18%	1.705%
3	1.648	88	92	100	rVB	114314	152198	15.22%	1.969%
4	2.294	192	198	209	rBV	190247	299540	29.95%	3.875%
5	2.392	209	214	219	rVB	7025	12790	1.28%	0.165%
6	2.489	229	230	234	rBV4	604	769	0.08%	0.010%
7	2.544	237	239	240	rBV2	919	770	0.08%	0.010%
8	2.563	240	242	248	rVB3	1471	1818	0.18%	0.024%
9	2.709	263	266	267	rBV2	613	602	0.06%	0.008%
10	2.782	274	278	281	rBV5	1242	2153	0.22%	0.028%
11	2.855	286	290	292	rBV3	778	1165	0.12%	0.015%
12	2.940	297	304	317	rVB2	11048	25823	2.58%	0.334%
13	3.111	331	332	334	rBV2	768	669	0.07%	0.009%
14	3.136	334	336	338	rVV2	670	661	0.07%	0.009%
15	3.172	340	342	344	rVB2	775	572	0.06%	0.007%
16	3.233	349	352	354	rBV	738	673	0.07%	0.009%
17	3.434	380	385	392	rVB4	3383	6913	0.69%	0.089%
18	3.526	399	400	402	rBV2	602	618	0.06%	0.008%
19	3.977	473	474	475	rVV	1035	454	0.05%	0.006%
20	3.995	475	477	480	rVB2	854	636	0.06%	0.008%
21	4.068	485	489	491	rVB3	734	993	0.10%	0.013%
22	4.105	491	495	498	rBV3	560	1113	0.11%	0.014%
23	4.166	503	505	506	rBV	652	522	0.05%	0.007%
24	4.398	540	543	545	rVB2	989	884	0.09%	0.011%
25	4.465	545	554	570	rBV	71369	218236	21.82%	2.824%
26	5.050	637	650	665	rBV2	135771	427662	42.76%	5.533%
27	5.208	674	676	678	rBV3	776	945	0.09%	0.012%
28	5.373	702	703	706	rBV2	686	605	0.06%	0.008%
29	5.464	716	718	721	rBV2	613	579	0.06%	0.007%
30	5.531	726	729	730	rBV2	505	543	0.05%	0.007%
31	5.550	730	732	734	rVV2	569	509	0.05%	0.007%
32	5.812	772	775	776	rBV2	506	462	0.05%	0.006%
33	5.964	789	800	813	rBV2	334668	1000123	100.00%	12.940%
34	6.355	856	864	873	rBV3	6626	18990	1.90%	0.246%
35	6.604	902	905	908	rBV3	638	762	0.08%	0.010%
36	6.665	914	915	919	rBV3	583	829	0.08%	0.011%

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Integrator: RTE

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Max Peaks: 100

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

37	6.757	921	930	947	rBV	242587	603082	60.30%	7.803%
38	7.062	978	980	981	rVB2	939	565	0.06%	0.007%
39	7.117	984	989	995	rVV7	2290	5931	0.59%	0.077%
40	7.306	1011	1020	1034	rBV	208282	469545	46.95%	6.075%
41	7.476	1044	1048	1051	rBV4	867	1100	0.11%	0.014%
42	7.598	1066	1068	1072	rBV5	496	676	0.07%	0.009%
43	7.659	1073	1078	1082	rBV	2563	4754	0.48%	0.062%
44	7.799	1096	1101	1115	rBV	77928	145049	14.50%	1.877%
45	8.324	1181	1187	1198	rBV	125448	213764	21.37%	2.766%
46	8.549	1219	1224	1234	rBV2	18553	35487	3.55%	0.459%
47	8.647	1234	1240	1258	rVV	474072	741227	74.11%	9.590%
48	8.897	1279	1281	1284	rBV3	558	775	0.08%	0.010%
49	8.952	1285	1290	1298	rBV2	98262	164234	16.42%	2.125%
50	9.244	1334	1338	1347	rBV	23758	37524	3.75%	0.485%
51	9.384	1356	1361	1373	rBV	305938	461962	46.19%	5.977%
52	9.488	1374	1378	1389	rVB	34141	53484	5.35%	0.692%
53	9.586	1389	1394	1402	rBV	17854	26725	2.67%	0.346%
54	9.695	1410	1412	1417	rBV3	1231	1268	0.13%	0.016%
55	9.787	1426	1427	1430	rBV2	629	552	0.06%	0.007%
56	9.915	1440	1448	1459	rBV	63568	90088	9.01%	1.166%
57	10.055	1465	1471	1488	rVB	492632	698524	69.84%	9.038%
58	10.195	1493	1494	1497	rVB3	651	461	0.05%	0.006%
59	10.250	1499	1503	1506	rBV4	856	1121	0.11%	0.015%
60	10.464	1536	1538	1541	rVV3	574	705	0.07%	0.009%
61	10.646	1565	1568	1572	rBV4	2196	2868	0.29%	0.037%
62	10.945	1615	1617	1618	rBV	692	477	0.05%	0.006%
63	11.000	1623	1626	1628	rVB2	605	765	0.08%	0.010%
64	11.189	1652	1657	1666	rVV	363031	482983	48.29%	6.249%
65	11.396	1690	1691	1694	rBV2	571	688	0.07%	0.009%
66	11.445	1697	1699	1701	rBV2	547	572	0.06%	0.007%
67	11.616	1726	1727	1730	rBV3	403	468	0.05%	0.006%
68	11.707	1739	1742	1743	rVB3	734	559	0.06%	0.007%
69	11.982	1784	1787	1788	rBV2	733	748	0.07%	0.010%
70	12.018	1788	1793	1803	rBV	416118	552635	55.26%	7.150%
71	12.317	1837	1842	1852	rBV	458785	588624	58.86%	7.616%
72	12.475	1866	1868	1871	rVB3	796	687	0.07%	0.009%
73	12.573	1881	1884	1885	rBV2	640	681	0.07%	0.009%
74	12.609	1888	1890	1893	rBV2	398	620	0.06%	0.008%
75	12.762	1914	1915	1919	rVB2	961	1070	0.11%	0.014%
76	12.811	1922	1923	1928	rVB2	666	770	0.08%	0.010%

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Peak separation: 5

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

77	12.853	1928	1930	1932	rBV2	840	795	0.08%	0.010%
78	12.872	1932	1933	1935	rBV2	569	449	0.04%	0.006%
79	13.109	1970	1972	1974	rBV3	701	886	0.09%	0.011%
80	13.274	1995	1999	2002	rVB3	670	992	0.10%	0.013%
81	13.304	2002	2004	2006	rBV2	490	544	0.05%	0.007%
82	13.884	2096	2099	2101	rBV2	406	552	0.06%	0.007%
83	14.067	2127	2129	2132	rVB2	650	497	0.05%	0.006%
84	14.121	2137	2138	2141	rBV3	503	485	0.05%	0.006%
85	14.341	2171	2174	2176	rBV3	688	747	0.07%	0.010%
86	14.451	2186	2192	2196	rBV4	1310	2147	0.21%	0.028%
87	14.518	2202	2203	2207	rVB3	654	482	0.05%	0.006%
88	14.566	2207	2211	2214	rBV4	757	960	0.10%	0.012%
89	14.597	2214	2216	2219	rVB2	852	829	0.08%	0.011%
90	14.640	2219	2223	2225	rBV4	616	954	0.10%	0.012%
91	14.877	2260	2262	2264	rVB2	773	525	0.05%	0.007%
92	14.987	2276	2280	2281	rBV3	757	849	0.08%	0.011%
93	15.103	2296	2299	2300	rBV2	642	601	0.06%	0.008%
94	15.182	2309	2312	2315	rVB3	643	752	0.08%	0.010%
95	15.414	2348	2350	2352	rBV3	574	565	0.06%	0.007%
96	15.865	2421	2424	2425	rBV2	945	705	0.07%	0.009%
97	15.883	2425	2427	2429	rBV3	636	668	0.07%	0.009%
98	16.127	2466	2467	2469	rBV2	679	524	0.05%	0.007%
99	16.481	2523	2525	2526	rBV	977	527	0.05%	0.007%
100	16.517	2529	2531	2532	rBV	751	582	0.06%	0.008%

Sum of corrected areas: 7729163

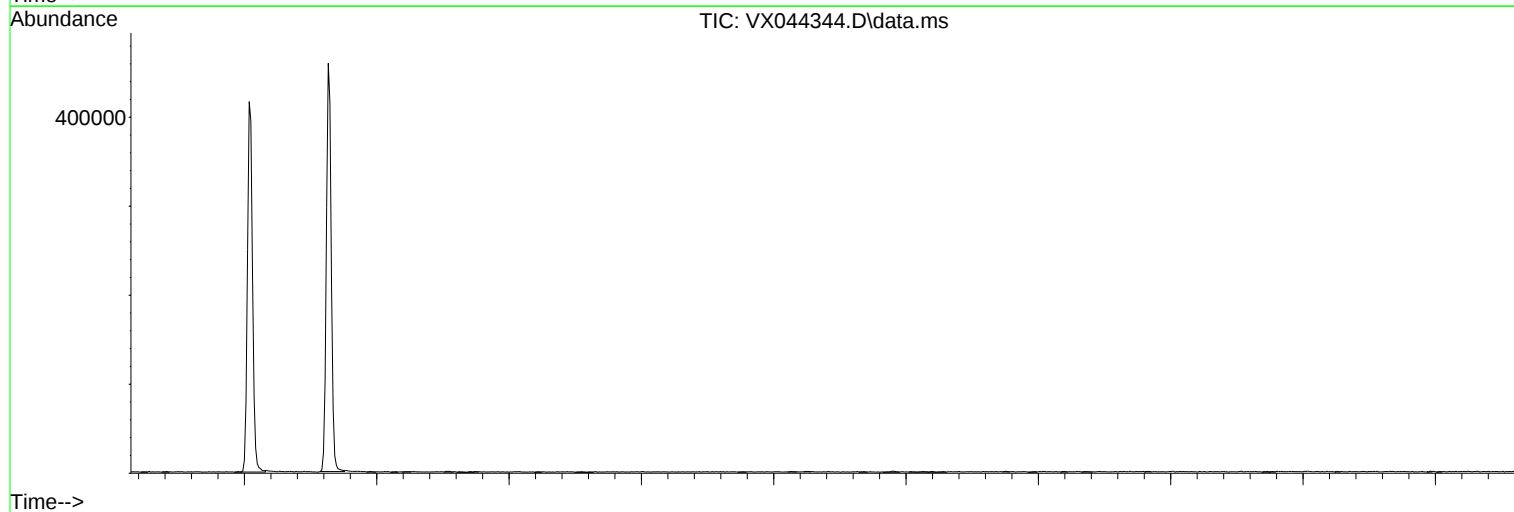
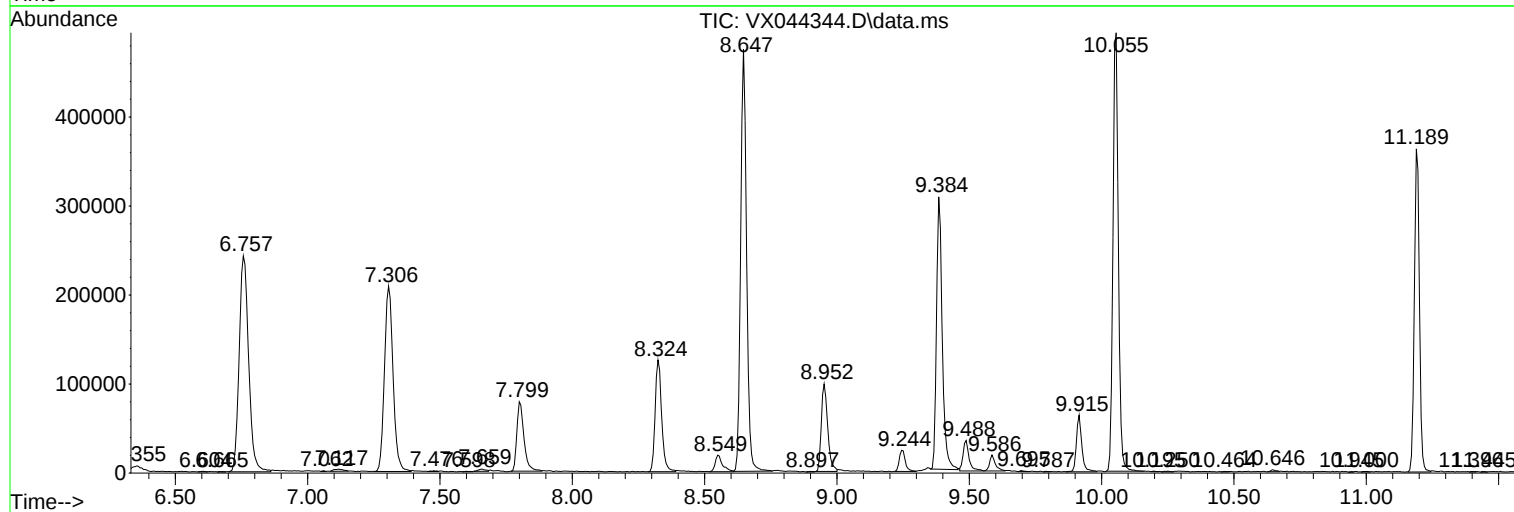
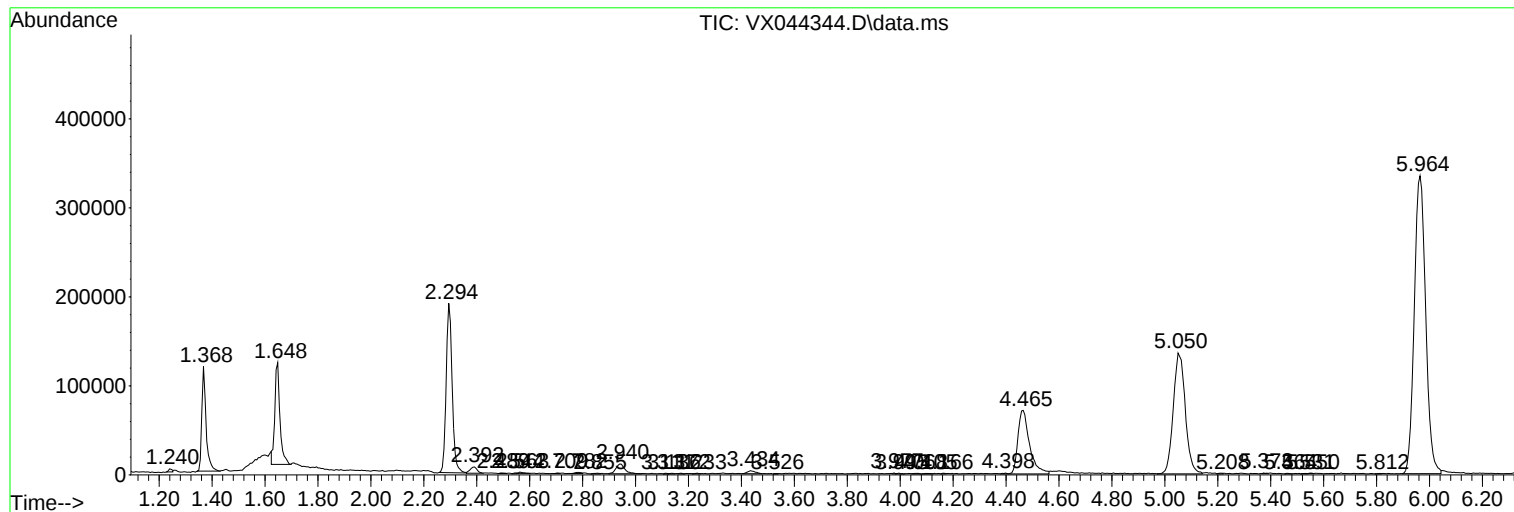
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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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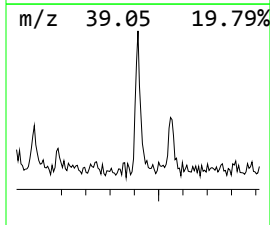
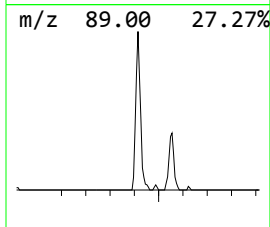
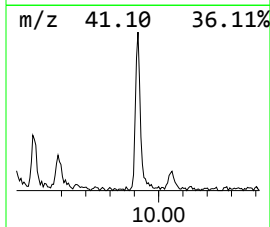
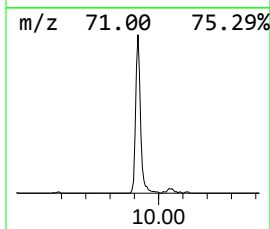
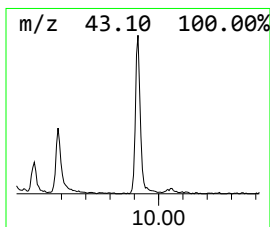
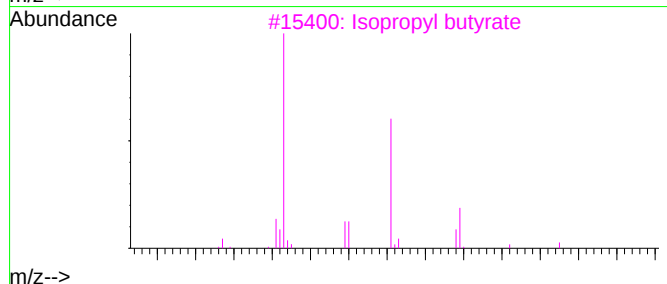
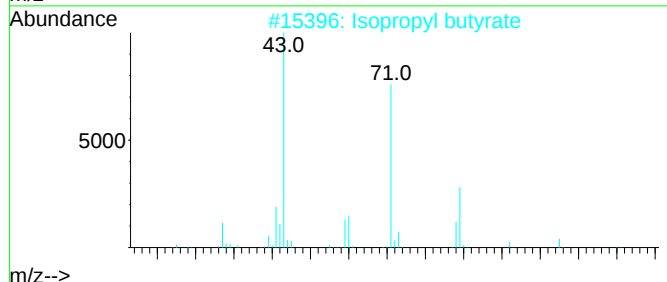
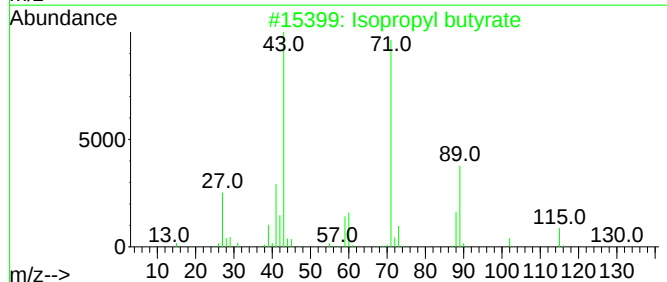
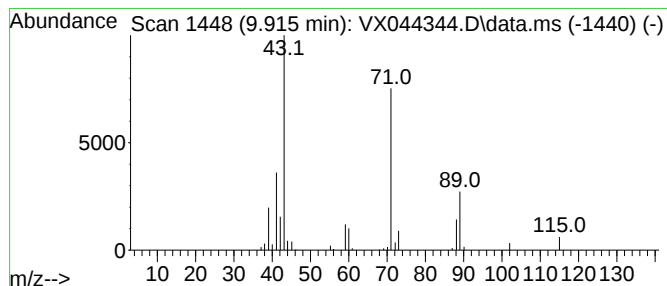
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

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	6.45 ug/L	90088	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	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
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	6.5	ug/L	90088	2	10.055	698524	50.0