

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044358.D
 Acq On : 17 Dec 2024 17:51
 Operator : JC/MD
 Sample : P5235-17 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AT4

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\SFAMXLM120524WMA.M
 Title : VOC Analysis

Signal : TIC: VX044358.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	23	25	27	rBV2	1843	2086	0.22%	0.028%
2	1.367	42	46	55	rBV	108609	122694	12.77%	1.636%
3	1.648	89	92	99	rVB	106014	130765	13.61%	1.744%
4	2.294	192	198	209	rBV	176370	281632	29.31%	3.756%
5	2.386	209	213	219	rVB2	6247	10027	1.04%	0.134%
6	2.556	237	241	246	rBV4	1314	2069	0.22%	0.028%
7	2.751	272	273	274	rBV	915	484	0.05%	0.006%
8	2.788	274	279	283	rVB5	1752	3454	0.36%	0.046%
9	2.898	293	297	298	rBV3	503	683	0.07%	0.009%
10	2.946	298	305	312	rVV	12858	29088	3.03%	0.388%
11	3.020	315	317	318	rBV2	529	486	0.05%	0.006%
12	3.306	363	364	365	rBV	1001	581	0.06%	0.008%
13	3.355	369	372	375	rVB3	878	950	0.10%	0.013%
14	3.434	381	385	388	rBV5	1797	3089	0.32%	0.041%
15	3.568	404	407	408	rBV2	788	809	0.08%	0.011%
16	3.983	473	475	477	rVV	752	654	0.07%	0.009%
17	4.032	481	483	485	rVB2	831	695	0.07%	0.009%
18	4.062	485	488	490	rBV3	505	613	0.06%	0.008%
19	4.080	490	491	494	rBV3	588	516	0.05%	0.007%
20	4.257	515	520	523	rBV4	888	1492	0.16%	0.020%
21	4.410	542	545	546	rBV3	626	572	0.06%	0.008%
22	4.458	546	553	566	rBV	67994	201550	20.98%	2.688%
23	4.721	594	596	598	rBV3	727	700	0.07%	0.009%
24	4.769	602	604	607	rBV4	666	739	0.08%	0.010%
25	4.849	616	617	620	rVB2	990	564	0.06%	0.008%
26	5.056	639	651	664	rBV	130947	403964	42.04%	5.387%
27	5.294	686	690	692	rVB2	755	814	0.08%	0.011%
28	5.964	789	800	821	rBV3	324990	960837	100.00%	12.814%
29	6.202	838	839	842	rVB2	782	622	0.06%	0.008%
30	6.232	842	844	848	rBV4	768	941	0.10%	0.013%
31	6.348	857	863	869	rBV4	5822	15262	1.59%	0.204%
32	6.464	881	882	885	rVV2	591	486	0.05%	0.006%
33	6.507	887	889	892	rVB3	782	715	0.07%	0.010%
34	6.592	901	903	906	rVB4	711	590	0.06%	0.008%
35	6.635	908	910	912	rBV	801	629	0.07%	0.008%
36	6.757	920	930	944	rBV	251762	607496	63.23%	8.102%

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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	7.123	984	990	995	rVV7	2739	6377	0.66%	0.085%
38	7.184	998	1000	1003	rVB2	593	564	0.06%	0.008%
39	7.305	1011	1020	1035	rBV	205229	452050	47.05%	6.029%
40	7.476	1046	1048	1050	rBV2	810	751	0.08%	0.010%
41	7.592	1063	1067	1074	rVV5	3143	7451	0.78%	0.099%
42	7.799	1095	1101	1115	rBV	83425	160744	16.73%	2.144%
43	8.068	1143	1145	1148	rBV3	1020	949	0.10%	0.013%
44	8.220	1169	1170	1173	rBV3	559	591	0.06%	0.008%
45	8.324	1181	1187	1201	rBV	119158	197636	20.57%	2.636%
46	8.470	1209	1211	1215	rBV3	643	673	0.07%	0.009%
47	8.549	1219	1224	1233	rBV2	16942	30042	3.13%	0.401%
48	8.647	1234	1240	1250	rBV	449438	698844	72.73%	9.320%
49	8.951	1284	1290	1300	rBV2	97675	161286	16.79%	2.151%
50	9.244	1332	1338	1345	rBV	24370	38693	4.03%	0.516%
51	9.342	1352	1354	1356	rBV3	3683	3063	0.32%	0.041%
52	9.384	1356	1361	1373	rBV	288684	446595	46.48%	5.956%
53	9.488	1374	1378	1382	rBV	34399	47581	4.95%	0.635%
54	9.586	1390	1394	1406	rVB2	23801	40651	4.23%	0.542%
55	9.915	1443	1448	1459	rBV	68772	98869	10.29%	1.319%
56	10.055	1465	1471	1484	rBV	501689	699572	72.81%	9.330%
57	10.250	1500	1503	1505	rVB3	654	679	0.07%	0.009%
58	10.287	1507	1509	1510	rBV	908	745	0.08%	0.010%
59	10.445	1534	1535	1540	rVB4	1015	1277	0.13%	0.017%
60	10.488	1540	1542	1544	rBV2	645	707	0.07%	0.009%
61	10.524	1544	1548	1550	rBV3	962	1511	0.16%	0.020%
62	10.646	1564	1568	1572	rVV3	4631	6907	0.72%	0.092%
63	10.707	1576	1578	1582	rVB2	750	669	0.07%	0.009%
64	10.817	1594	1596	1599	rBV2	551	661	0.07%	0.009%
65	10.963	1618	1620	1622	rBV2	487	539	0.06%	0.007%
66	11.036	1630	1632	1636	rVV3	534	667	0.07%	0.009%
67	11.189	1652	1657	1668	rVV	358142	463699	48.26%	6.184%
68	11.341	1681	1682	1684	rVB2	1090	496	0.05%	0.007%
69	11.360	1684	1685	1687	rBV	960	708	0.07%	0.009%
70	11.457	1699	1701	1703	rVV	843	534	0.06%	0.007%
71	11.506	1707	1709	1712	rVB2	1017	796	0.08%	0.011%
72	11.542	1712	1715	1716	rBV2	703	610	0.06%	0.008%
73	11.634	1726	1730	1731	rBV2	471	492	0.05%	0.007%
74	11.707	1740	1742	1747	rVB3	850	805	0.08%	0.011%
75	11.805	1756	1758	1761	rVB2	452	518	0.05%	0.007%
76	11.896	1771	1773	1776	rBV2	576	518	0.05%	0.007%

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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\SFAMXLM120524WMA.M
 Title : VOC Analysis

77	11.927	1776	1778	1781	rBV4	658	702	0.07%	0.009%
78	12.018	1788	1793	1803	rBV	412321	549515	57.19%	7.328%
79	12.317	1837	1842	1851	rBV	453093	563950	58.69%	7.521%
80	12.762	1911	1915	1916	rBV2	1003	1154	0.12%	0.015%
81	12.884	1929	1935	1936	rBV4	1161	1618	0.17%	0.022%
82	13.085	1966	1968	1969	rBV2	547	514	0.05%	0.007%
83	13.121	1970	1974	1978	rVB2	1180	1888	0.20%	0.025%
84	13.158	1978	1980	1982	rBV2	843	879	0.09%	0.012%
85	13.225	1988	1991	1992	rBV2	523	486	0.05%	0.006%
86	13.512	2036	2038	2041	rVB3	1133	919	0.10%	0.012%
87	13.652	2057	2061	2064	rVB2	631	866	0.09%	0.012%
88	13.701	2064	2069	2070	rBV2	725	693	0.07%	0.009%
89	13.853	2092	2094	2096	rVB2	753	640	0.07%	0.009%
90	13.884	2096	2099	2100	rBV	984	912	0.09%	0.012%
91	14.085	2130	2132	2133	rBV	584	491	0.05%	0.007%
92	14.140	2136	2141	2142	rVV3	1212	1597	0.17%	0.021%
93	14.341	2173	2174	2176	rBV2	652	590	0.06%	0.008%
94	14.487	2195	2198	2200	rBV2	610	735	0.08%	0.010%
95	14.670	2225	2228	2230	rBV2	762	602	0.06%	0.008%
96	14.713	2233	2235	2237	rBV2	658	545	0.06%	0.007%
97	15.725	2400	2401	2404	rVB3	790	506	0.05%	0.007%
98	16.084	2459	2460	2466	rVB4	980	1216	0.13%	0.016%
99	16.377	2507	2508	2510	rBV2	799	583	0.06%	0.008%
100	16.596	2542	2544	2548	rBV2	845	997	0.10%	0.013%

Sum of corrected areas: 7498466

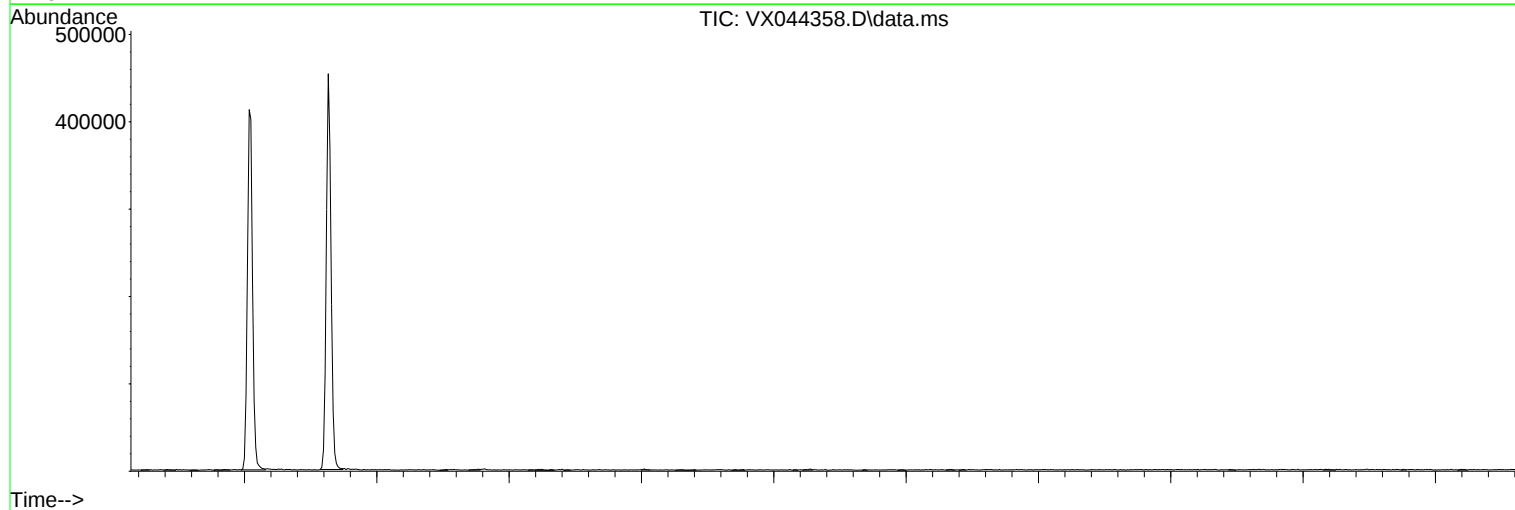
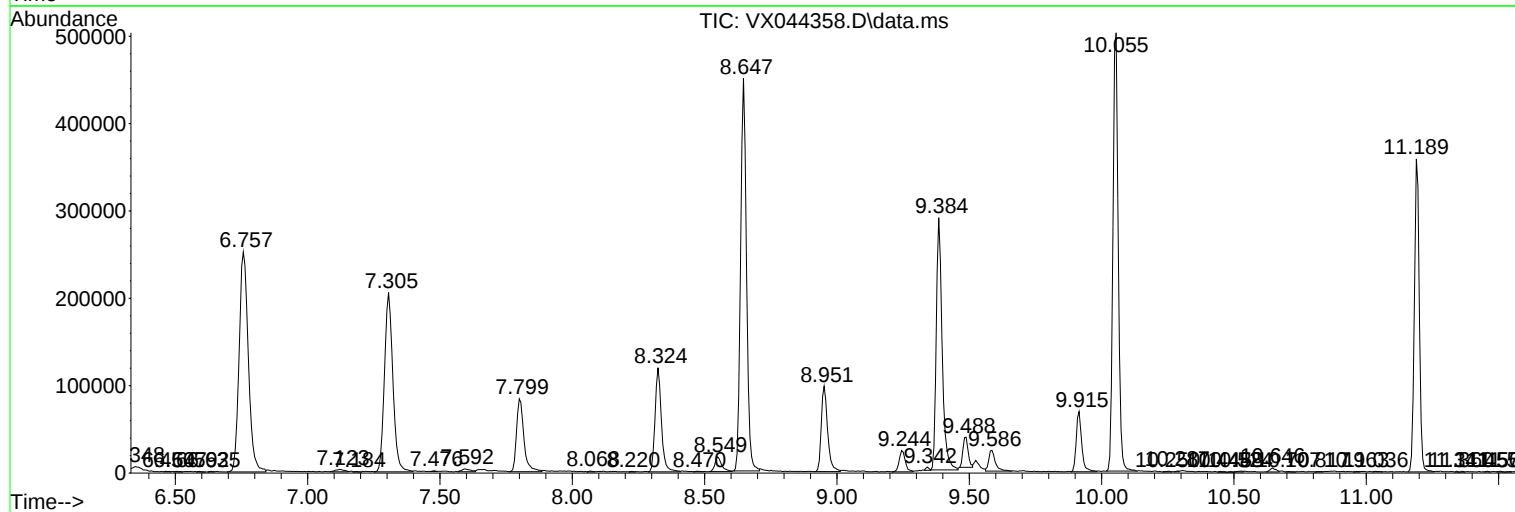
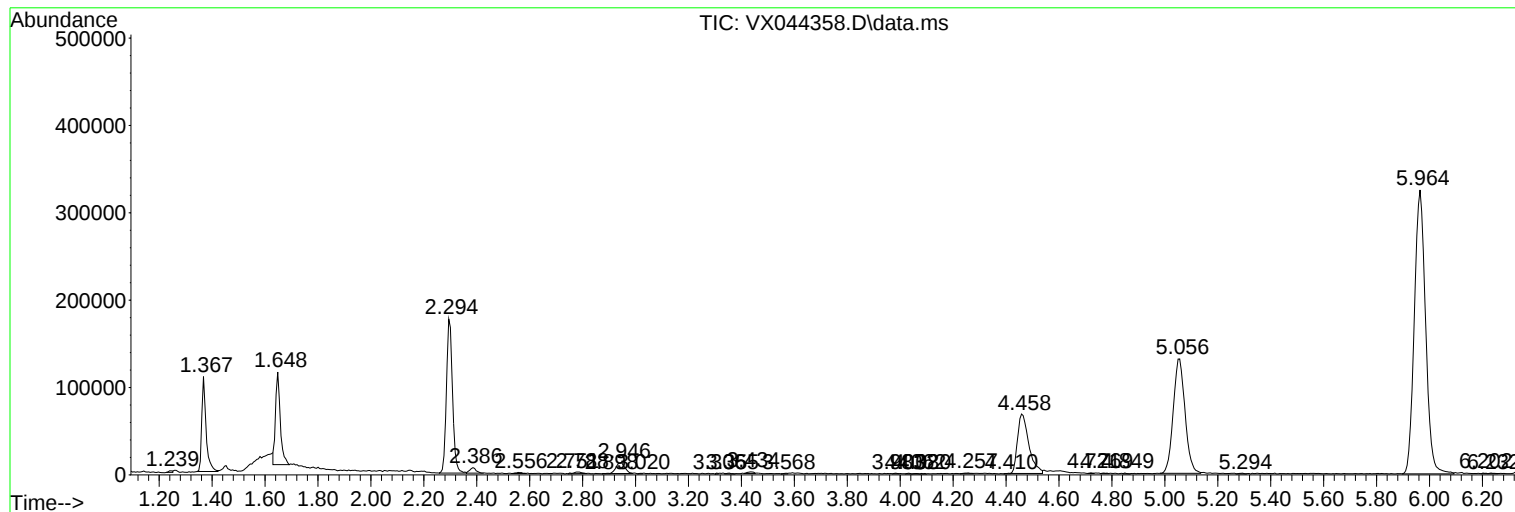
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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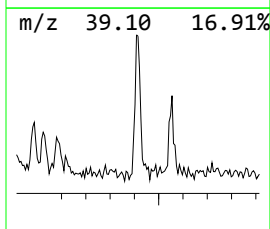
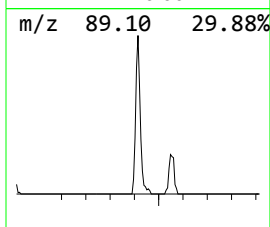
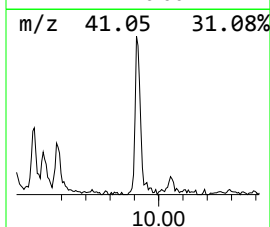
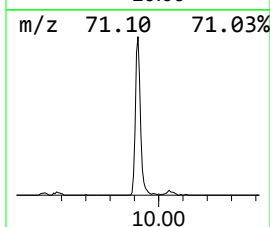
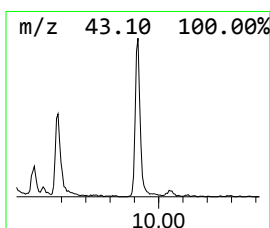
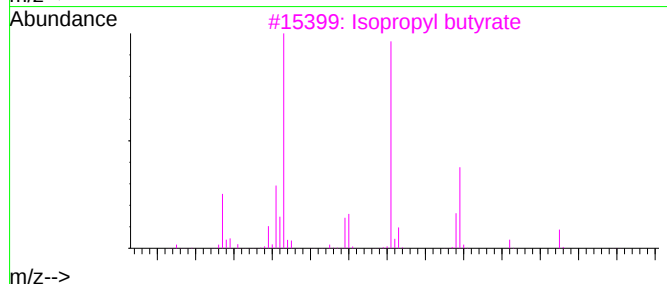
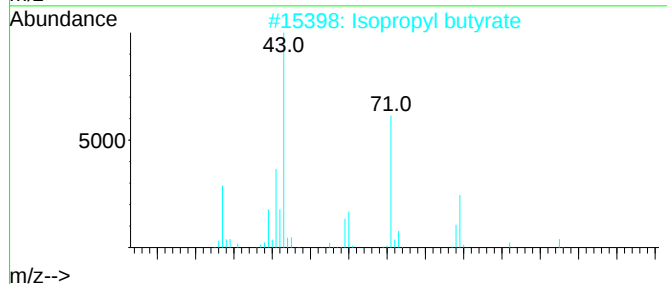
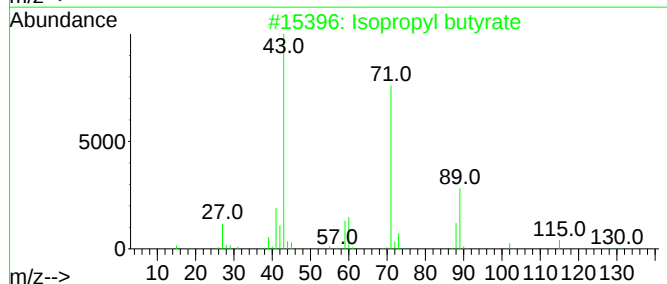
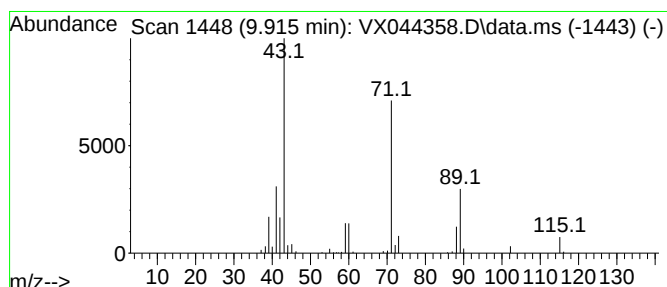
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	7.07 ug/L	98869	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	90
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	78
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isopropyl butyrate	9.915	7.1	ug/L	98869	2	10.055	699572	50.0