

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044347.D
 Acq On : 17 Dec 2024 13:32
 Operator : JC/MD
 Sample : P5235-06 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AT5

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\SFAMXML120524WMA.M
 Title : VOC Analysis

Signal : TIC: VX044347.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	23	26	27	rBV	2835	3183	0.31%	0.040%
2	1.368	42	46	54	rBV	124933	135043	13.22%	1.708%
3	1.447	57	59	63	rBV	3512	3483	0.34%	0.044%
4	1.648	88	92	99	rVB	107401	149252	14.61%	1.888%
5	2.294	192	198	209	rBV	189127	301592	29.52%	3.815%
6	2.386	209	213	224	rVB	9289	16677	1.63%	0.211%
7	2.562	237	242	251	rVB4	2229	4047	0.40%	0.051%
8	2.788	274	279	283	rVB5	2198	4112	0.40%	0.052%
9	2.940	297	304	314	rVV2	15909	38246	3.74%	0.484%
10	3.038	317	320	322	rBV3	709	731	0.07%	0.009%
11	3.148	336	338	340	rBV3	523	585	0.06%	0.007%
12	3.434	379	385	392	rVV6	2675	6149	0.60%	0.078%
13	3.593	409	411	416	rVV3	866	1329	0.13%	0.017%
14	4.056	483	487	489	rVB3	618	667	0.07%	0.008%
15	4.093	489	493	494	rBV2	470	730	0.07%	0.009%
16	4.148	499	502	503	rVB2	828	627	0.06%	0.008%
17	4.166	503	505	508	rBV3	424	631	0.06%	0.008%
18	4.233	514	516	518	rVB2	775	709	0.07%	0.009%
19	4.257	518	520	523	rBV3	780	944	0.09%	0.012%
20	4.385	537	541	542	rBV2	522	710	0.07%	0.009%
21	4.458	545	553	569	rBV	74525	222950	21.82%	2.820%
22	4.897	623	625	630	rVV2	961	1120	0.11%	0.014%
23	5.056	640	651	668	rBV2	136498	429610	42.05%	5.434%
24	5.263	681	685	687	rVB2	604	673	0.07%	0.009%
25	5.617	740	743	746	rBV3	1131	1044	0.10%	0.013%
26	5.964	789	800	826	rBV2	345342	1021753	100.00%	12.924%
27	6.233	841	844	848	rBV4	703	896	0.09%	0.011%
28	6.348	858	863	877	rBV2	5914	16920	1.66%	0.214%
29	6.550	894	896	899	rBV2	726	917	0.09%	0.012%
30	6.757	921	930	948	rBV	229276	566204	55.41%	7.162%
31	7.062	975	980	981	rBV2	877	1076	0.11%	0.014%
32	7.110	984	988	989	rBV3	2523	3283	0.32%	0.042%
33	7.306	1011	1020	1035	rBV	219505	475045	46.49%	6.009%
34	7.653	1075	1077	1083	rVB2	2437	3680	0.36%	0.047%
35	7.799	1095	1101	1115	rBV	74640	140301	13.73%	1.775%
36	8.275	1176	1179	1181	rBV3	908	1138	0.11%	0.014%

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 Title : VOC Analysis

37	8.324	1181	1187	1197	rVV	132677	215214	21.06%	2.722%
38	8.549	1219	1224	1233	rBV	18578	33969	3.32%	0.430%
39	8.647	1234	1240	1256	rVB	477234	755573	73.95%	9.557%
40	8.952	1285	1290	1307	rVV2	99109	160165	15.68%	2.026%
41	9.159	1321	1324	1325	rBV2	578	697	0.07%	0.009%
42	9.244	1332	1338	1345	rBV	26563	40302	3.94%	0.510%
43	9.305	1347	1348	1349	rVV	1351	891	0.09%	0.011%
44	9.342	1352	1354	1356	rVV3	4741	5337	0.52%	0.068%
45	9.384	1356	1361	1374	rVV	324999	494823	48.43%	6.259%
46	9.488	1374	1378	1389	rVV	35494	56578	5.54%	0.716%
47	9.586	1390	1394	1402	rVB2	12580	19624	1.92%	0.248%
48	9.768	1421	1424	1425	rBV2	659	832	0.08%	0.011%
49	9.915	1443	1448	1460	rVV	69811	93527	9.15%	1.183%
50	10.055	1465	1471	1486	rVB	468415	671680	65.74%	8.496%
51	10.195	1489	1494	1502	rVB	26928	36909	3.61%	0.467%
52	10.299	1506	1511	1518	rBV	45821	64606	6.32%	0.817%
53	10.457	1534	1537	1540	rVB2	782	942	0.09%	0.012%
54	10.494	1540	1543	1544	rBV2	584	647	0.06%	0.008%
55	10.646	1563	1568	1573	rBV2	13905	22141	2.17%	0.280%
56	10.738	1581	1583	1585	rBV3	869	792	0.08%	0.010%
57	10.963	1618	1620	1625	rBV4	447	630	0.06%	0.008%
58	11.189	1652	1657	1669	rBV	386779	495271	48.47%	6.264%
59	11.335	1678	1681	1682	rBV2	569	583	0.06%	0.007%
60	11.439	1694	1698	1699	rBV3	517	779	0.08%	0.010%
61	11.457	1699	1701	1704	rVV	1006	818	0.08%	0.010%
62	11.500	1706	1708	1710	rVB2	687	572	0.06%	0.007%
63	11.762	1749	1751	1757	rVB3	928	1476	0.14%	0.019%
64	12.018	1788	1793	1802	rBV	400946	526123	51.49%	6.655%
65	12.244	1827	1830	1831	rBV3	659	725	0.07%	0.009%
66	12.317	1837	1842	1851	rBV	471323	604458	59.16%	7.645%
67	12.524	1873	1876	1880	rVB4	528	702	0.07%	0.009%
68	12.762	1912	1915	1919	rVV2	1481	1889	0.18%	0.024%
69	12.792	1919	1920	1925	rVV3	809	801	0.08%	0.010%
70	12.853	1928	1930	1933	rVV2	1031	1208	0.12%	0.015%
71	12.902	1936	1938	1944	rVV4	1335	2180	0.21%	0.028%
72	13.164	1978	1981	1984	rBB2	516	766	0.07%	0.010%
73	13.195	1984	1986	1989	rBV2	548	578	0.06%	0.007%
74	13.335	2005	2009	2015	rVB5	5816	9396	0.92%	0.119%
75	13.390	2015	2018	2021	rBV2	485	569	0.06%	0.007%
76	13.426	2021	2024	2027	rBV4	2352	2784	0.27%	0.035%

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

77	13.512	2035	2038	2043	rVB5	2520	2990	0.29%	0.038%
78	13.695	2064	2068	2070	rVV3	762	824	0.08%	0.010%
79	13.731	2070	2074	2075	rVV3	423	637	0.06%	0.008%
80	13.749	2075	2077	2080	rVV4	545	635	0.06%	0.008%
81	13.792	2080	2084	2086	rVV2	536	785	0.08%	0.010%
82	13.847	2091	2093	2096	rVB3	750	840	0.08%	0.011%
83	13.969	2111	2113	2117	rBV2	735	857	0.08%	0.011%
84	14.097	2128	2134	2135	rBV3	970	1122	0.11%	0.014%
85	14.176	2145	2147	2150	rVB2	1027	832	0.08%	0.011%
86	14.237	2154	2157	2159	rVV3	697	635	0.06%	0.008%
87	14.310	2167	2169	2172	rBV	854	827	0.08%	0.010%
88	14.347	2172	2175	2178	rBV3	452	610	0.06%	0.008%
89	14.451	2187	2192	2197	rBV5	998	2040	0.20%	0.026%
90	14.493	2197	2199	2203	rVB3	556	715	0.07%	0.009%
91	14.603	2216	2217	2219	rBV2	749	632	0.06%	0.008%
92	15.200	2313	2315	2319	rVV5	678	907	0.09%	0.011%
93	15.249	2321	2323	2326	rVV3	734	602	0.06%	0.008%
94	15.322	2333	2335	2337	rBV2	680	719	0.07%	0.009%
95	15.542	2370	2371	2373	rBV2	797	659	0.06%	0.008%
96	15.908	2429	2431	2433	rVB2	776	695	0.07%	0.009%
97	15.938	2433	2436	2438	rBV3	823	944	0.09%	0.012%
98	16.023	2447	2450	2455	rBV4	915	1651	0.16%	0.021%
99	16.310	2495	2497	2499	rBV2	586	669	0.07%	0.008%
100	16.511	2526	2530	2532	rBV2	479	721	0.07%	0.009%

Sum of corrected areas: 7906162

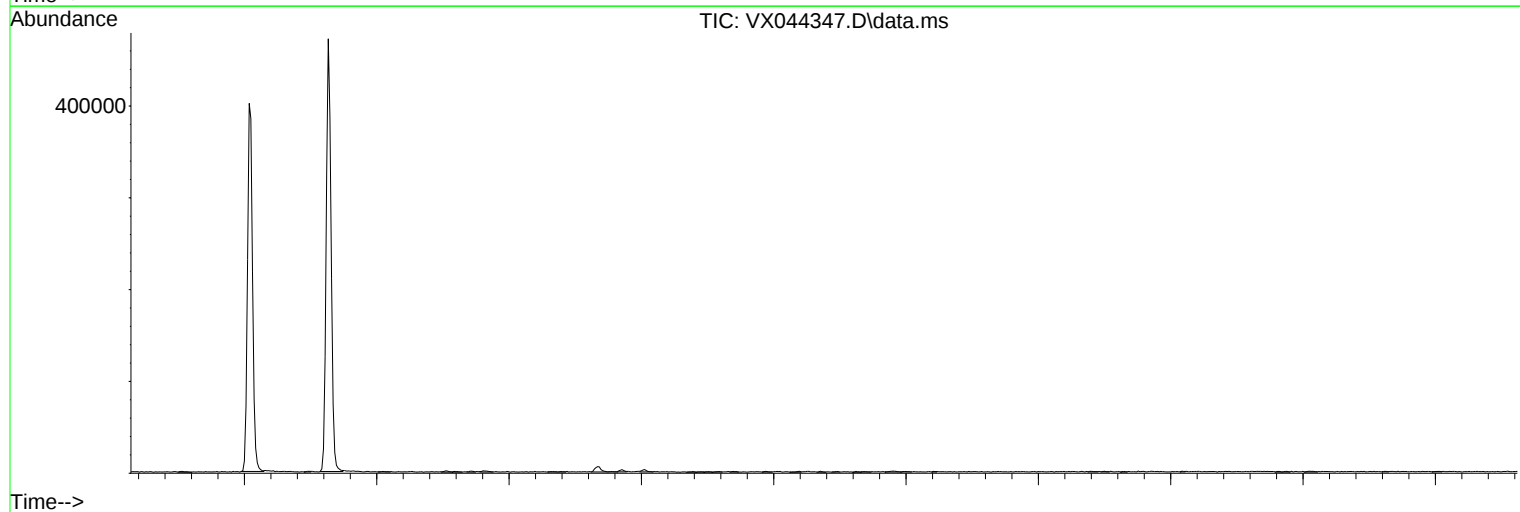
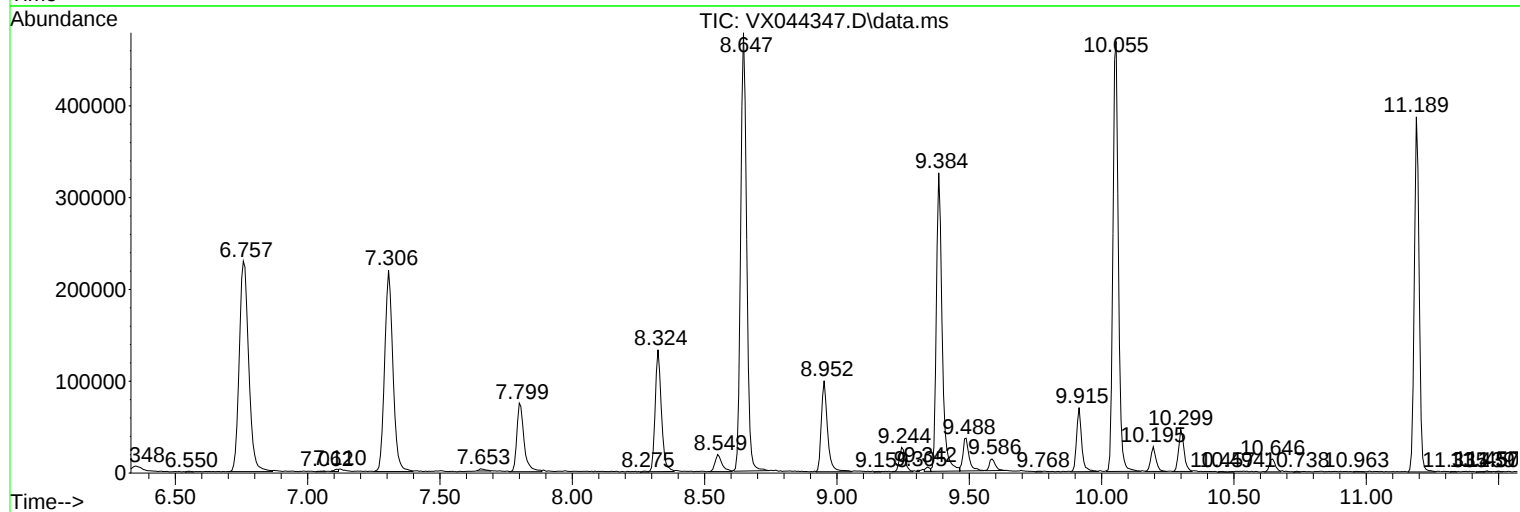
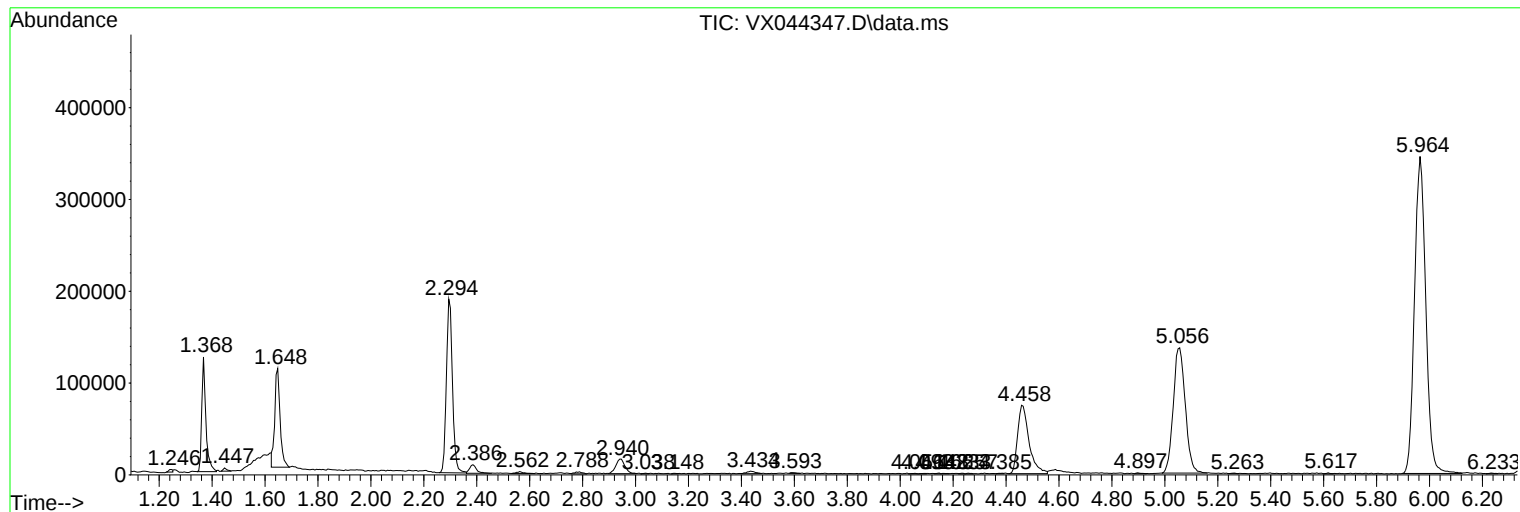
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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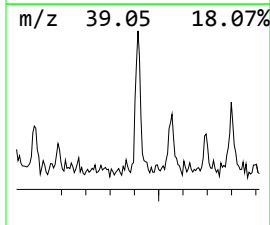
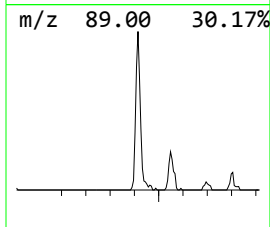
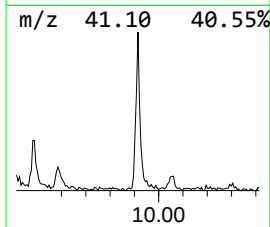
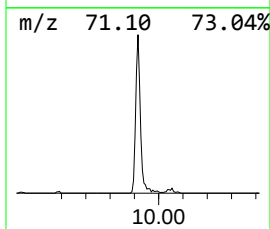
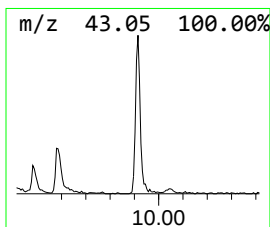
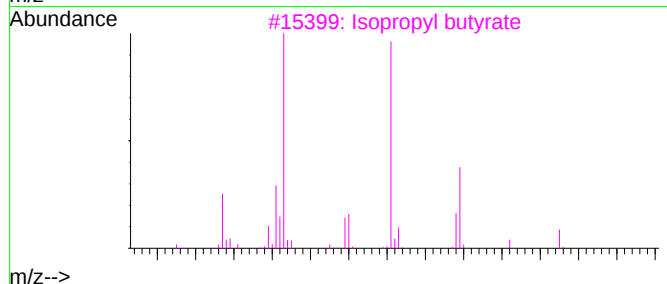
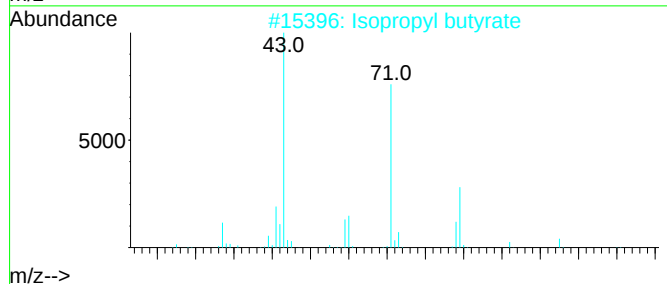
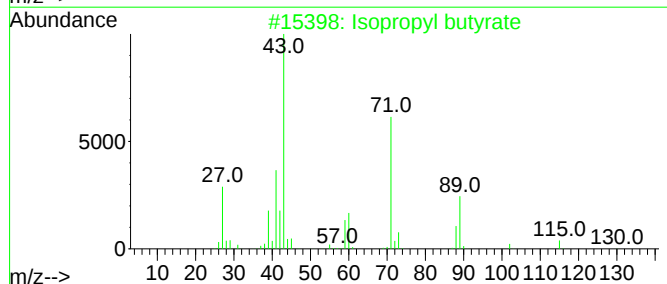
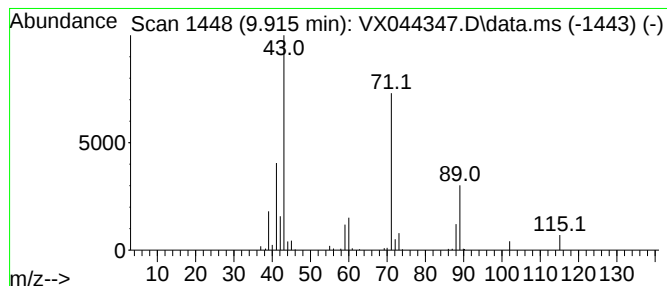
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	6.96 ug/L	93527	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	83
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



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Quant Title : VOC Analysis

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl butyrate	9.915	7.0	ug/L	93527	2	10.055	671680	50.0