

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012825\
 Data File : VX044748.D
 Acq On : 28 Jan 2025 16:44
 Operator : JC/MD
 Sample : PB166233TB 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VLEB233

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: VX044748.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	22	25	35	rBV	14762	27106	2.44%	0.304%
2	1.367	42	46	58	rBV	139838	158840	14.28%	1.781%
3	1.648	88	92	101	rVB	75539	92099	8.28%	1.032%
4	2.294	192	198	208	rBV	218561	354323	31.85%	3.972%
5	2.386	209	213	223	rVB	6389	10719	0.96%	0.120%
6	2.696	262	264	269	rBV2	296	411	0.04%	0.005%
7	2.782	274	278	286	rVB4	1094	2242	0.20%	0.025%
8	2.855	289	290	292	rBV	568	490	0.04%	0.005%
9	2.940	298	304	311	rBV2	5171	11307	1.02%	0.127%
10	3.032	315	319	321	rBV3	485	739	0.07%	0.008%
11	3.087	324	328	331	rBV3	665	861	0.08%	0.010%
12	3.160	339	340	343	rVB2	538	457	0.04%	0.005%
13	3.282	356	360	361	rBV2	396	508	0.05%	0.006%
14	3.306	361	364	365	rVV2	347	409	0.04%	0.005%
15	3.324	365	367	370	rVV3	461	483	0.04%	0.005%
16	3.434	382	385	391	rVV4	1120	2535	0.23%	0.028%
17	3.507	394	397	398	rBV2	359	361	0.03%	0.004%
18	3.580	405	409	421	rVB4	2230	6217	0.56%	0.070%
19	4.074	487	490	493	rVB2	337	361	0.03%	0.004%
20	4.111	494	496	500	rVV2	446	425	0.04%	0.005%
21	4.288	523	525	527	rBV2	555	358	0.03%	0.004%
22	4.379	539	540	543	rBV2	608	581	0.05%	0.007%
23	4.458	545	553	572	rBV2	67303	217940	19.59%	2.443%
24	4.763	602	603	608	rBV3	720	930	0.08%	0.010%
25	5.050	638	650	667	rBV	136766	431928	38.83%	4.842%
26	5.263	684	685	689	rVB2	494	417	0.04%	0.005%
27	5.306	689	692	694	rBV2	282	480	0.04%	0.005%
28	5.550	730	732	734	rBV2	541	459	0.04%	0.005%
29	5.665	747	751	752	rBV3	525	519	0.05%	0.006%
30	5.964	789	800	820	rBV2	370228	1112323	100.00%	12.469%
31	6.251	845	847	850	rVB2	612	515	0.05%	0.006%
32	6.348	855	863	876	rBV2	8730	26096	2.35%	0.293%
33	6.757	921	930	948	rBV	296044	724161	65.10%	8.118%
34	7.116	984	989	990	rBV3	1061	1356	0.12%	0.015%
35	7.196	1000	1002	1005	rBV3	515	729	0.07%	0.008%
36	7.305	1011	1020	1036	rBV	228115	507312	45.61%	5.687%

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Integrator: RTE

Smoothing : OFF

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Max Peaks: 100

Peak Location: TOP

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 Title : VOC Analysis

37	7.519	1053	1055	1061	rBV5	722	1101	0.10%	0.012%
38	7.598	1066	1068	1070	rVB2	393	395	0.04%	0.004%
39	7.659	1073	1078	1082	rBV	3494	6243	0.56%	0.070%
40	7.799	1095	1101	1120	rBV	113770	216745	19.49%	2.430%
41	8.061	1142	1144	1147	rBV3	369	400	0.04%	0.004%
42	8.269	1177	1178	1181	rBV2	370	403	0.04%	0.005%
43	8.324	1181	1187	1199	rBV	162277	277515	24.95%	3.111%
44	8.549	1219	1224	1233	rVB	26648	44014	3.96%	0.493%
45	8.647	1233	1240	1258	rBV	525657	882961	79.38%	9.898%
46	8.951	1284	1290	1309	rBV2	142121	233862	21.02%	2.621%
47	9.183	1327	1328	1330	rBV2	439	348	0.03%	0.004%
48	9.244	1333	1338	1347	rVV	43470	64495	5.80%	0.723%
49	9.342	1347	1354	1356	rVV3	6951	12439	1.12%	0.139%
50	9.384	1356	1361	1373	rVV	260399	429076	38.57%	4.810%
51	9.482	1373	1377	1386	rVV	63976	97560	8.77%	1.094%
52	9.579	1389	1393	1407	rVB	38046	59614	5.36%	0.668%
53	9.872	1440	1441	1442	rBV	473	329	0.03%	0.004%
54	9.909	1442	1447	1462	rVV	124021	173212	15.57%	1.942%
55	10.049	1465	1470	1493	rVB	561109	843751	75.85%	9.458%
56	10.354	1517	1520	1522	rBV2	561	517	0.05%	0.006%
57	10.524	1544	1548	1555	rVB5	1073	2004	0.18%	0.022%
58	10.646	1563	1568	1575	rBV2	8149	13495	1.21%	0.151%
59	11.104	1641	1643	1645	rBV	636	367	0.03%	0.004%
60	11.189	1652	1657	1665	rBV	386864	495930	44.59%	5.559%
61	11.591	1719	1723	1724	rBV3	364	471	0.04%	0.005%
62	11.628	1727	1729	1731	rBV	345	362	0.03%	0.004%
63	11.756	1747	1750	1757	rVB4	654	1148	0.10%	0.013%
64	11.908	1774	1775	1779	rVB	528	486	0.04%	0.005%
65	11.975	1779	1786	1788	rBV4	1216	2017	0.18%	0.023%
66	12.018	1788	1793	1807	rBV	530673	691906	62.20%	7.756%
67	12.317	1837	1842	1862	rVB	513909	650377	58.47%	7.290%
68	12.500	1870	1872	1873	rBV2	662	357	0.03%	0.004%
69	12.573	1880	1884	1885	rBV	320	373	0.03%	0.004%
70	12.762	1912	1915	1918	rBV2	745	988	0.09%	0.011%
71	12.835	1925	1927	1931	rVB2	326	349	0.03%	0.004%
72	12.957	1944	1947	1950	rBV3	313	414	0.04%	0.005%
73	13.115	1971	1973	1975	rBV2	384	503	0.05%	0.006%
74	13.170	1980	1982	1984	rVV2	480	412	0.04%	0.005%
75	13.188	1984	1985	1988	rVB	375	321	0.03%	0.004%
76	13.298	2000	2003	2004	rVB2	375	354	0.03%	0.004%

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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\SFAMXML012825WMA.M
 Title : VOC Analysis

77	13.432	2023	2025	2029	rVB2	476	499	0.04%	0.006%
78	13.475	2029	2032	2033	rBV2	386	340	0.03%	0.004%
79	13.506	2036	2037	2040	rVB	515	338	0.03%	0.004%
80	13.591	2049	2051	2052	rBV2	646	539	0.05%	0.006%
81	13.664	2061	2063	2065	rBV2	413	407	0.04%	0.005%
82	13.743	2073	2076	2078	rBV2	443	385	0.03%	0.004%
83	13.786	2078	2083	2087	rBV5	1226	2566	0.23%	0.029%
84	13.908	2101	2103	2104	rBV	379	371	0.03%	0.004%
85	14.036	2118	2124	2125	rBV2	446	685	0.06%	0.008%
86	14.127	2137	2139	2144	rVB3	2000	2401	0.22%	0.027%
87	14.170	2144	2146	2147	rBV	375	317	0.03%	0.004%
88	14.298	2166	2167	2172	rBV2	312	397	0.04%	0.004%
89	14.463	2192	2194	2197	rBV3	329	380	0.03%	0.004%
90	14.530	2203	2205	2210	rVB3	498	795	0.07%	0.009%
91	14.578	2210	2213	2214	rBV2	449	355	0.03%	0.004%
92	14.597	2214	2216	2219	rBB3	411	428	0.04%	0.005%
93	14.664	2225	2227	2230	rBV2	329	342	0.03%	0.004%
94	14.737	2237	2239	2241	rVB2	488	323	0.03%	0.004%
95	14.767	2241	2244	2245	rBV2	536	410	0.04%	0.005%
96	15.078	2293	2295	2297	rBV2	449	441	0.04%	0.005%
97	15.389	2341	2346	2350	rBV4	1365	1957	0.18%	0.022%
98	16.182	2475	2476	2478	rVB	614	344	0.03%	0.004%
99	16.237	2482	2485	2489	rBV4	523	883	0.08%	0.010%
100	16.316	2497	2498	2500	rBV2	660	432	0.04%	0.005%

Sum of corrected areas: 8920946

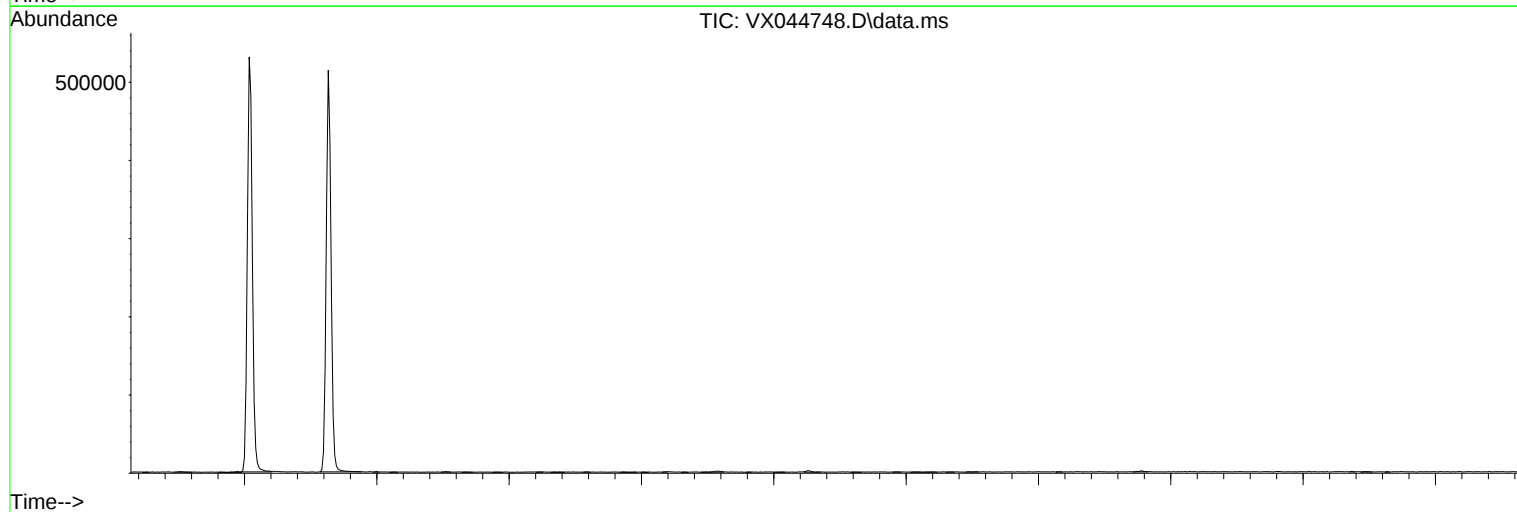
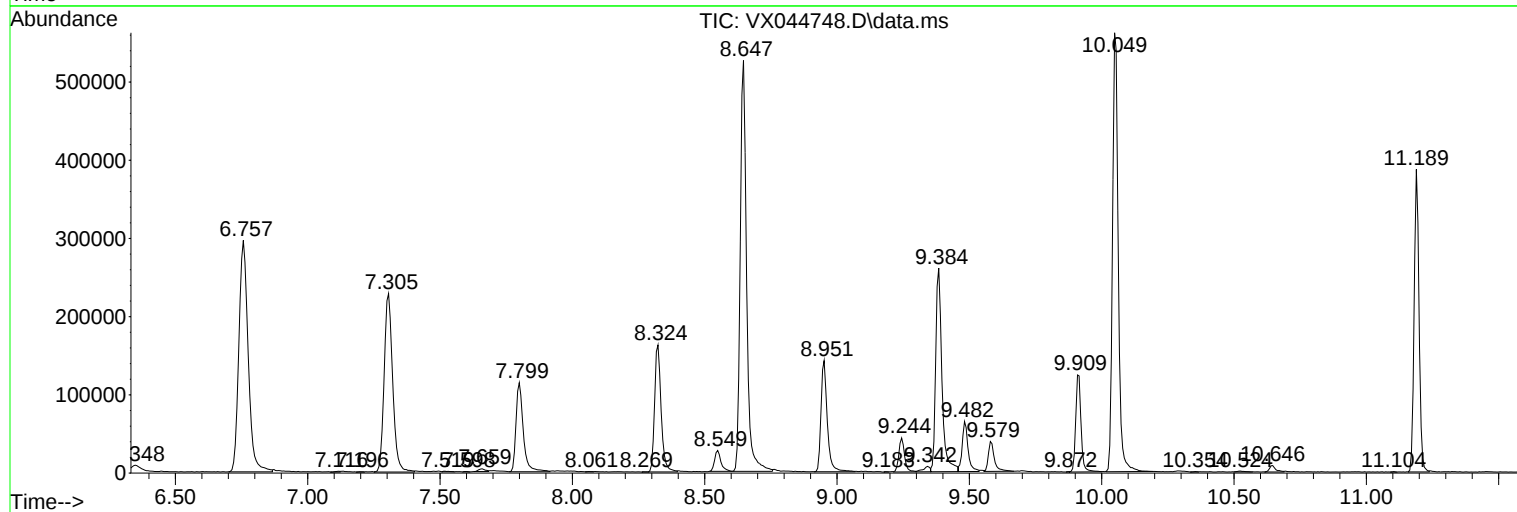
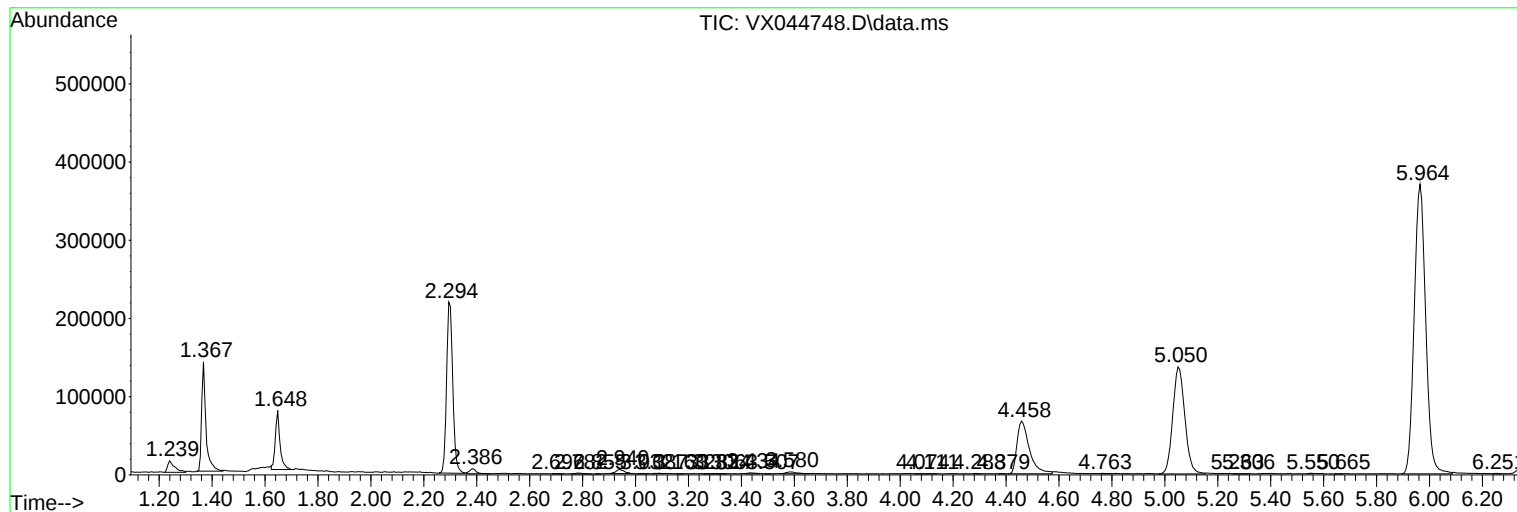
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ALS Vial : 14 Sample Multiplier: 1

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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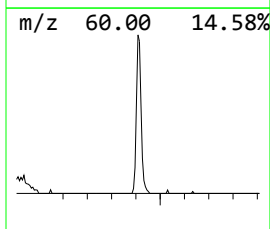
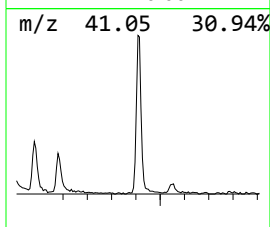
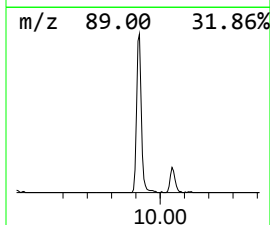
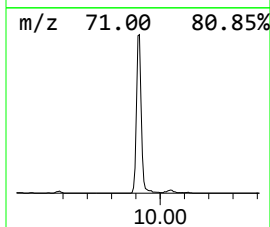
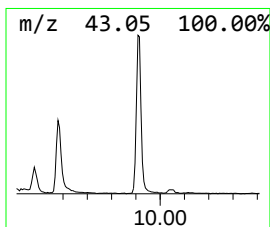
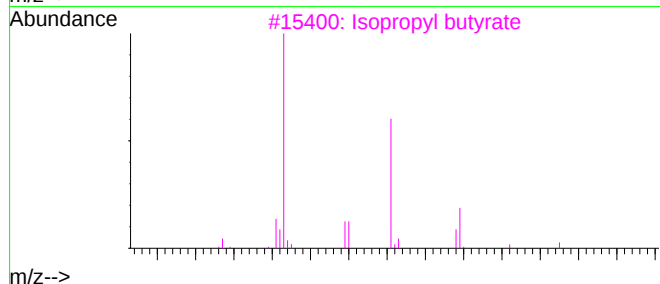
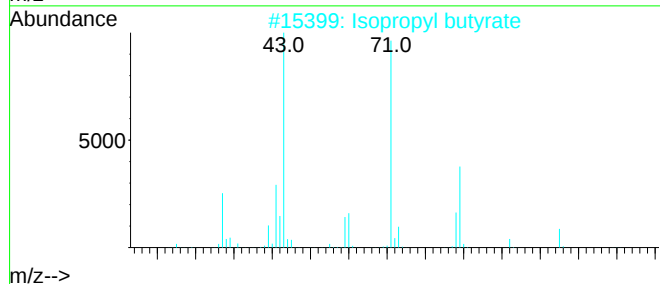
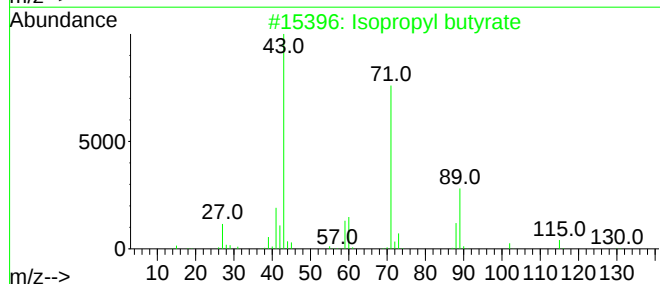
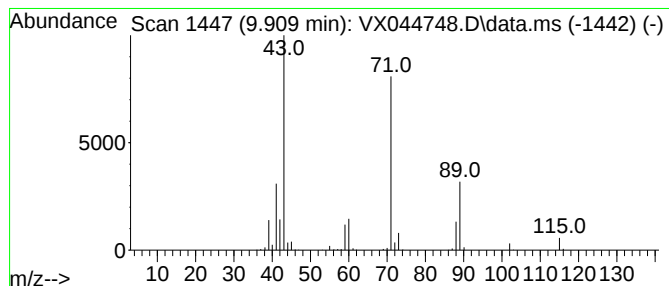
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.909	10.26 ug/L	173212	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	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	9.909	10.3	ug/L	173212	2	10.049	843751	50.0