

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044350.D
 Acq On : 17 Dec 2024 14:42
 Operator : JC/MD
 Sample : P5235-11 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AW1

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: VX044350.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	2940	2959	0.30%	0.039%
2	1.368	42	46	57	rBV	118168	129512	13.30%	1.713%
3	1.648	88	92	100	rVB	115209	157113	16.14%	2.078%
4	2.294	192	198	209	rVB	184866	291848	29.97%	3.860%
5	2.630	251	253	255	rVV2	838	591	0.06%	0.008%
6	2.739	269	271	273	rBV2	606	558	0.06%	0.007%
7	2.788	274	279	284	rVB6	1976	3177	0.33%	0.042%
8	2.861	289	291	293	rBV2	732	574	0.06%	0.008%
9	2.941	298	304	312	rVB	5902	14774	1.52%	0.195%
10	3.056	321	323	326	rBV3	586	686	0.07%	0.009%
11	3.191	342	345	346	rVV3	521	505	0.05%	0.007%
12	3.325	365	367	370	rVB4	576	646	0.07%	0.009%
13	3.434	380	385	389	rVV4	2432	4901	0.50%	0.065%
14	3.581	407	409	412	rBV4	441	509	0.05%	0.007%
15	3.623	414	416	418	rVB2	664	513	0.05%	0.007%
16	3.660	418	422	424	rBV5	676	768	0.08%	0.010%
17	3.721	428	432	433	rVB3	583	574	0.06%	0.008%
18	3.745	433	436	437	rBV2	634	641	0.07%	0.008%
19	3.886	456	459	461	rBV3	508	747	0.08%	0.010%
20	4.087	490	492	495	rVB2	616	600	0.06%	0.008%
21	4.288	523	525	529	rBV3	597	779	0.08%	0.010%
22	4.465	546	554	572	rBV	69490	207402	21.30%	2.743%
23	4.757	600	602	604	rBV3	1223	989	0.10%	0.013%
24	4.904	623	626	628	rBV3	453	544	0.06%	0.007%
25	4.971	635	637	639	rBV2	540	504	0.05%	0.007%
26	5.056	639	651	671	rVV2	131129	414866	42.61%	5.487%
27	5.349	697	699	701	rBV3	521	607	0.06%	0.008%
28	5.446	714	715	720	rVB3	568	584	0.06%	0.008%
29	5.550	728	732	733	rBV2	916	1137	0.12%	0.015%
30	5.690	753	755	756	rBV2	500	434	0.04%	0.006%
31	5.708	756	758	760	rVV2	438	478	0.05%	0.006%
32	5.964	789	800	812	rBV2	330210	973650	100.00%	12.878%
33	6.361	858	865	877	rVV4	5735	17471	1.79%	0.231%
34	6.574	898	900	903	rVB2	562	478	0.05%	0.006%
35	6.757	921	930	948	rBV	255453	614023	63.06%	8.122%
36	7.104	983	987	988	rBV3	2248	2923	0.30%	0.039%

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Integration Parameters: LSCINT.P

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	7.208	1002	1004	1007	rVB3	1025	741	0.08%	0.010%
38	7.306	1011	1020	1037	rVV	203749	453964	46.62%	6.004%
39	7.464	1045	1046	1048	rBV2	472	475	0.05%	0.006%
40	7.556	1060	1061	1063	rBV2	469	418	0.04%	0.006%
41	7.653	1073	1077	1078	rBV3	2688	3582	0.37%	0.047%
42	7.806	1096	1102	1114	rBV	57912	109845	11.28%	1.453%
43	7.952	1124	1126	1130	rBV4	816	1083	0.11%	0.014%
44	8.025	1136	1138	1141	rVB2	1048	979	0.10%	0.013%
45	8.171	1158	1162	1163	rBV4	765	669	0.07%	0.009%
46	8.257	1175	1176	1178	rBV	557	476	0.05%	0.006%
47	8.324	1181	1187	1199	rVV	119824	203179	20.87%	2.687%
48	8.549	1219	1224	1234	rBV	18926	34031	3.50%	0.450%
49	8.647	1234	1240	1253	rVV	462249	719351	73.88%	9.515%
50	8.952	1285	1290	1302	rBV2	90756	146963	15.09%	1.944%
51	9.244	1334	1338	1346	rVV	25337	38940	4.00%	0.515%
52	9.342	1346	1354	1356	rVV4	3732	7810	0.80%	0.103%
53	9.385	1356	1361	1373	rVV	299419	464773	47.74%	6.147%
54	9.482	1374	1377	1390	rVV	26039	45775	4.70%	0.605%
55	9.592	1390	1395	1404	rVB2	6485	12268	1.26%	0.162%
56	9.842	1433	1436	1437	rBV3	723	693	0.07%	0.009%
57	9.915	1443	1448	1456	rBV	66716	89443	9.19%	1.183%
58	10.055	1465	1471	1483	rBV	506002	714855	73.42%	9.455%
59	10.336	1515	1517	1519	rVB	616	422	0.04%	0.006%
60	10.439	1532	1534	1537	rBV3	419	468	0.05%	0.006%
61	10.525	1547	1548	1553	rVB2	1121	1162	0.12%	0.015%
62	10.653	1566	1569	1573	rBV3	1450	2573	0.26%	0.034%
63	10.799	1589	1593	1594	rBV2	495	544	0.06%	0.007%
64	10.884	1605	1607	1610	rBV2	645	830	0.09%	0.011%
65	10.951	1615	1618	1622	rVB3	459	701	0.07%	0.009%
66	11.073	1633	1638	1640	rBV5	554	673	0.07%	0.009%
67	11.146	1648	1650	1651	rBV2	521	432	0.04%	0.006%
68	11.189	1652	1657	1667	rVV	362620	471215	48.40%	6.233%
69	11.305	1674	1676	1677	rBV2	665	623	0.06%	0.008%
70	11.457	1698	1701	1703	rBV3	524	751	0.08%	0.010%
71	11.799	1754	1757	1759	rBV3	628	901	0.09%	0.012%
72	12.018	1788	1793	1802	rBV	445579	569427	58.48%	7.532%
73	12.317	1837	1842	1856	rVB	461746	589629	60.56%	7.799%
74	12.500	1870	1872	1875	rBV3	525	536	0.06%	0.007%
75	12.805	1918	1922	1923	rBV2	456	459	0.05%	0.006%
76	12.957	1945	1947	1953	rVB2	894	1059	0.11%	0.014%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Stop Thrs : 0

Peak Location: TOP

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

77	13.000	1953	1954	1957	rBV2	491	556	0.06%	0.007%
78	13.231	1990	1992	1993	rVB	906	500	0.05%	0.007%
79	13.244	1993	1994	1998	rBV2	695	694	0.07%	0.009%
80	13.280	1998	2000	2001	rBV2	808	615	0.06%	0.008%
81	13.433	2022	2025	2027	rBV3	584	797	0.08%	0.011%
82	13.731	2073	2074	2077	rBV2	497	457	0.05%	0.006%
83	13.798	2084	2085	2090	rVB4	624	500	0.05%	0.007%
84	13.963	2110	2112	2117	rVV2	553	836	0.09%	0.011%
85	14.054	2125	2127	2131	rBV2	741	751	0.08%	0.010%
86	14.128	2135	2139	2144	rVV5	1217	2344	0.24%	0.031%
87	14.262	2158	2161	2164	rBV2	648	720	0.07%	0.010%
88	14.347	2174	2175	2178	rBV2	452	471	0.05%	0.006%
89	14.628	2219	2221	2222	rBV2	484	449	0.05%	0.006%
90	15.286	2327	2329	2331	rBV2	525	496	0.05%	0.007%
91	15.585	2376	2378	2380	rVB2	792	506	0.05%	0.007%
92	15.621	2380	2384	2387	rBV3	526	1024	0.11%	0.014%
93	15.707	2397	2398	2400	rBV2	517	417	0.04%	0.006%
94	15.932	2433	2435	2437	rBV2	761	699	0.07%	0.009%
95	16.048	2453	2454	2457	rBV3	1109	1077	0.11%	0.014%
96	16.078	2457	2459	2464	rVV4	623	1061	0.11%	0.014%
97	16.207	2478	2480	2483	rVB3	703	664	0.07%	0.009%
98	16.237	2483	2485	2489	rBV4	794	1164	0.12%	0.015%
99	16.517	2529	2531	2534	rBV3	691	1039	0.11%	0.014%
100	16.664	2553	2555	2559	rVB3	792	803	0.08%	0.011%

Sum of corrected areas: 7560423

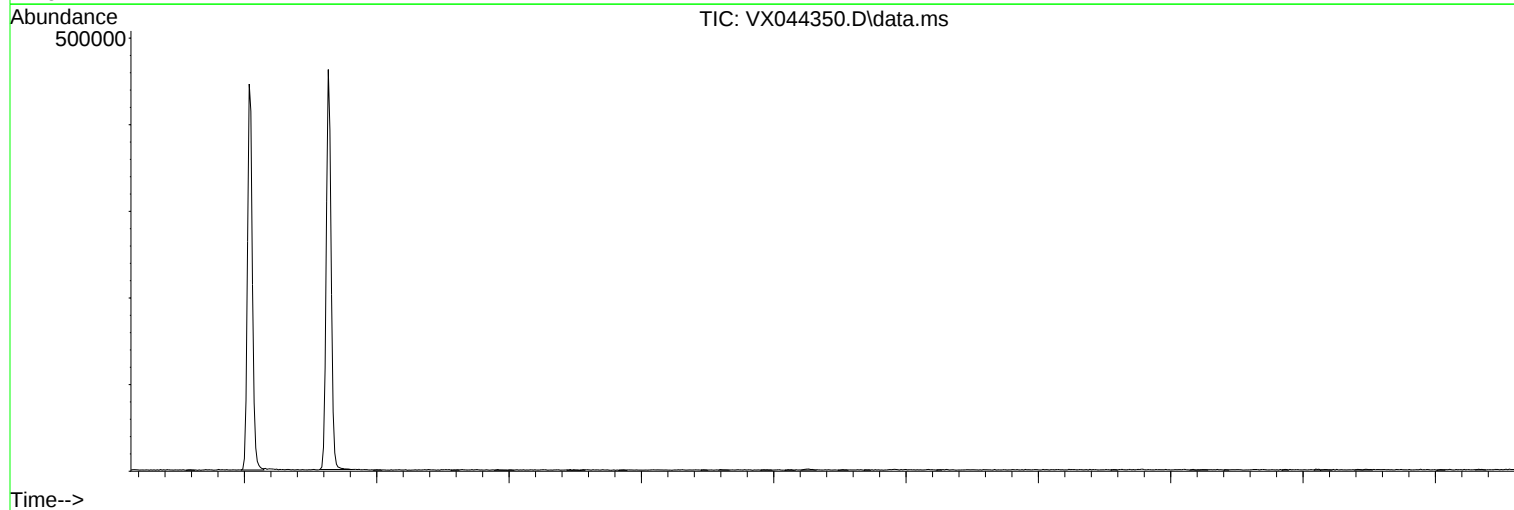
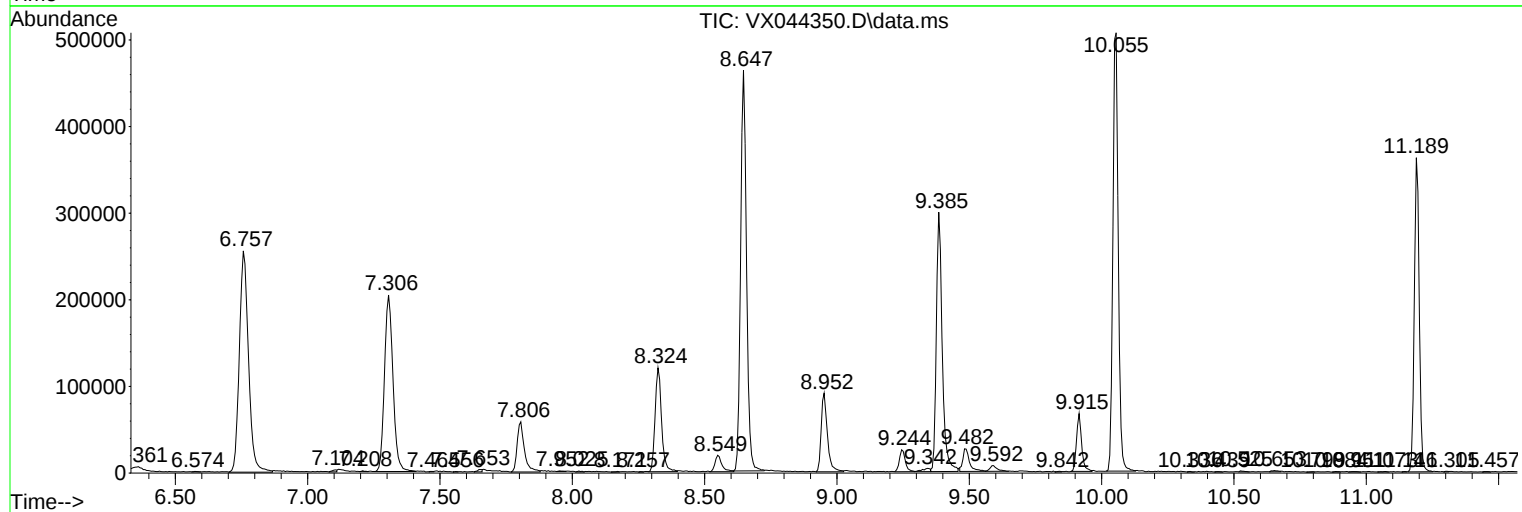
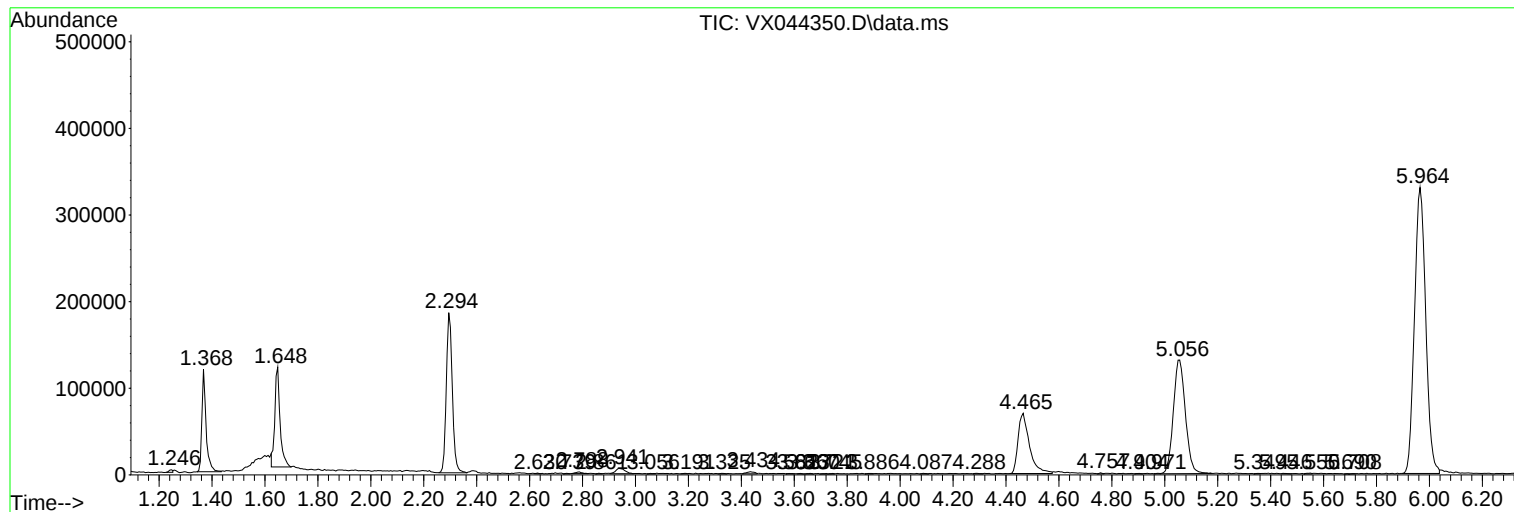
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ALS Vial : 17 Sample Multiplier: 1

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 Title : VOC Analysis

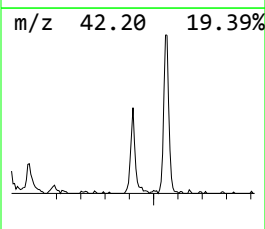
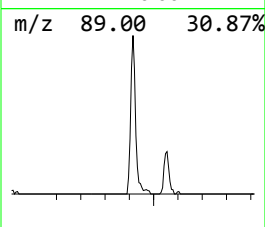
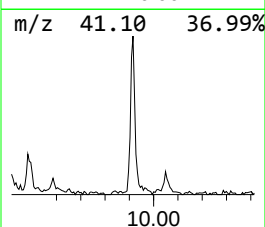
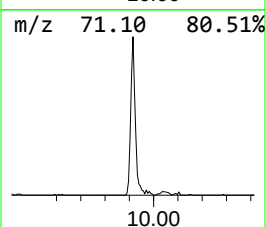
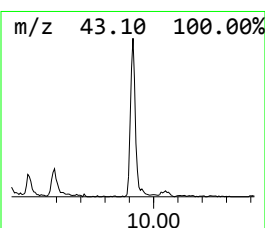
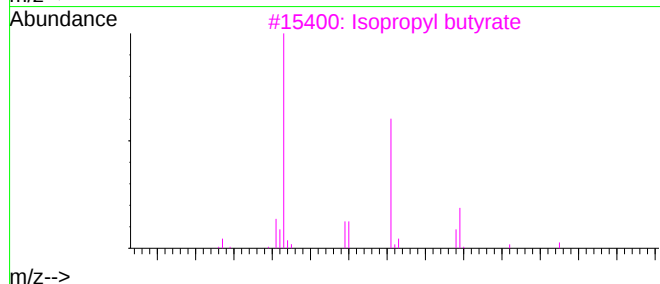
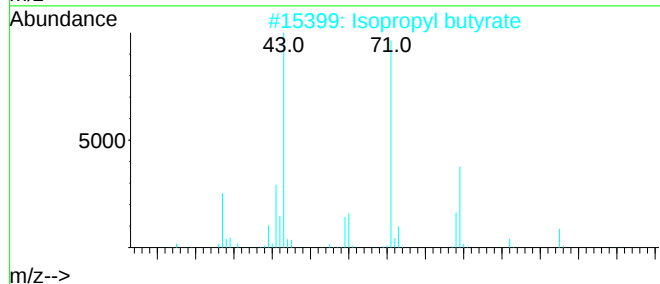
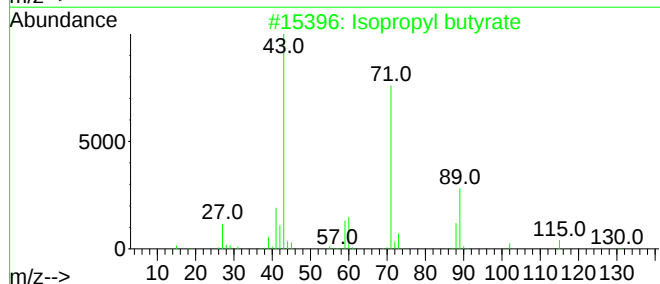
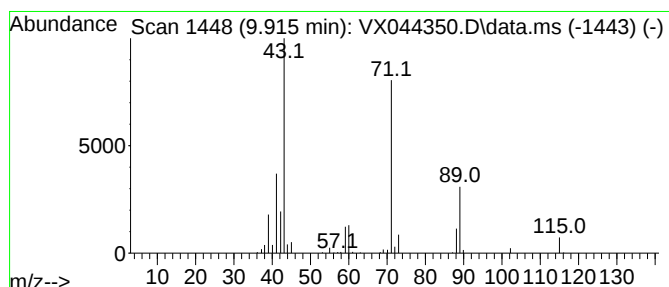
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	6.26 ug/L	89443	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	80
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	72
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl butyrate	9.915	6.3	ug/L	89443	2	10.055	714855	50.0