

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044345.D
 Acq On : 17 Dec 2024 12:45
 Operator : JC/MD
 Sample : P5235-04 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AT2

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: VX044345.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	3149	3609	0.36%	0.046%
2	1.368	42	46	55	rBV	121256	134807	13.29%	1.736%
3	1.648	89	92	99	rVB	110455	136614	13.47%	1.759%
4	2.294	192	198	209	rBV	186079	305205	30.08%	3.930%
5	2.386	209	213	220	rVB	4499	6712	0.66%	0.086%
6	2.697	263	264	266	rBV2	954	606	0.06%	0.008%
7	2.782	274	278	280	rBV4	1478	1969	0.19%	0.025%
8	2.843	286	288	292	rVB3	796	665	0.07%	0.009%
9	2.934	297	303	304	rBV2	5185	6631	0.65%	0.085%
10	3.142	332	337	339	rBV4	509	869	0.09%	0.011%
11	3.270	356	358	361	rVB3	554	518	0.05%	0.007%
12	3.367	370	374	377	rVB3	664	888	0.09%	0.011%
13	3.434	377	385	393	rBV7	2554	7101	0.70%	0.091%
14	3.757	436	438	441	rVB2	564	535	0.05%	0.007%
15	3.861	452	455	458	rBV3	672	915	0.09%	0.012%
16	3.928	465	466	471	rBV	663	630	0.06%	0.008%
17	4.020	479	481	483	rBV2	592	565	0.06%	0.007%
18	4.117	496	497	500	rVV2	980	599	0.06%	0.008%
19	4.245	515	518	520	rBV3	695	997	0.10%	0.013%
20	4.312	527	529	531	rBV3	872	931	0.09%	0.012%
21	4.330	531	532	536	rVB2	802	515	0.05%	0.007%
22	4.458	545	553	569	rBV	72345	216562	21.35%	2.789%
23	4.745	597	600	601	rBV3	556	557	0.05%	0.007%
24	4.952	630	634	636	rVB2	631	956	0.09%	0.012%
25	5.056	638	651	670	rVV	136361	434160	42.80%	5.591%
26	5.379	700	704	705	rBV2	1246	1162	0.11%	0.015%
27	5.397	705	707	710	rVB3	854	1053	0.10%	0.014%
28	5.544	728	731	732	rBV2	827	913	0.09%	0.012%
29	5.623	743	744	748	rBV3	415	479	0.05%	0.006%
30	5.964	789	800	818	rBV2	339976	1014488	100.00%	13.064%
31	6.172	832	834	835	rBV	811	634	0.06%	0.008%
32	6.208	838	840	841	rBV2	501	470	0.05%	0.006%
33	6.263	847	849	851	rBV2	436	472	0.05%	0.006%
34	6.348	856	863	878	rBV5	6093	19299	1.90%	0.249%
35	6.757	921	930	946	rBV	253305	615361	60.66%	7.924%
36	7.031	973	975	979	rVB3	671	693	0.07%	0.009%

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 Title : VOC Analysis

37	7.104	984	987	988	rBV3	1844	2067	0.20%	0.027%
38	7.306	1012	1020	1035	rBV	215940	472452	46.57%	6.084%
39	7.653	1073	1077	1079	rBV2	3074	4581	0.45%	0.059%
40	7.799	1096	1101	1114	rBV	60151	114203	11.26%	1.471%
41	8.324	1181	1187	1202	rVV	124742	216282	21.32%	2.785%
42	8.421	1202	1203	1206	rVV2	1217	1061	0.10%	0.014%
43	8.464	1208	1210	1213	rVB4	969	1060	0.10%	0.014%
44	8.549	1219	1224	1232	rBV2	18382	31683	3.12%	0.408%
45	8.647	1234	1240	1254	rVV	477276	742706	73.21%	9.564%
46	8.952	1285	1290	1299	rBV2	94292	151438	14.93%	1.950%
47	9.098	1312	1314	1315	rBV	717	666	0.07%	0.009%
48	9.159	1321	1324	1326	rBV2	635	653	0.06%	0.008%
49	9.244	1333	1338	1346	rBV	26246	40251	3.97%	0.518%
50	9.342	1346	1354	1356	rVV4	3658	7531	0.74%	0.097%
51	9.384	1356	1361	1373	rVV	309542	483358	47.65%	6.224%
52	9.488	1374	1378	1391	rVV	26036	45631	4.50%	0.588%
53	9.586	1391	1394	1404	rVB	8362	12962	1.28%	0.167%
54	9.872	1439	1441	1442	rBV	599	530	0.05%	0.007%
55	9.915	1443	1448	1458	rVV	64722	86884	8.56%	1.119%
56	10.055	1465	1471	1485	rBV	503383	722704	71.24%	9.306%
57	10.195	1492	1494	1497	rVB4	876	745	0.07%	0.010%
58	10.494	1539	1543	1544	rBV2	780	1128	0.11%	0.015%
59	10.512	1544	1546	1547	rBV2	720	470	0.05%	0.006%
60	10.653	1564	1569	1571	rBV4	1702	2465	0.24%	0.032%
61	10.787	1590	1591	1593	rVB	907	517	0.05%	0.007%
62	10.854	1599	1602	1605	rVV3	695	931	0.09%	0.012%
63	10.909	1609	1611	1614	rBV4	641	723	0.07%	0.009%
64	11.000	1623	1626	1627	rBV2	578	483	0.05%	0.006%
65	11.049	1631	1634	1635	rBV2	715	602	0.06%	0.008%
66	11.189	1651	1657	1668	rBV	376671	487226	48.03%	6.274%
67	11.317	1677	1678	1682	rVB3	880	764	0.08%	0.010%
68	11.451	1696	1700	1702	rBV3	523	637	0.06%	0.008%
69	11.811	1757	1759	1761	rBV2	786	490	0.05%	0.006%
70	12.018	1788	1793	1807	rBV	457171	580184	57.19%	7.471%
71	12.317	1837	1842	1853	rBV	482819	608897	60.02%	7.841%
72	12.963	1947	1948	1953	rVB2	799	850	0.08%	0.011%
73	13.012	1953	1956	1958	rVV2	668	853	0.08%	0.011%
74	13.036	1958	1960	1961	rVV2	687	524	0.05%	0.007%
75	13.055	1961	1963	1964	rVV2	605	512	0.05%	0.007%
76	13.103	1968	1971	1974	rVV3	571	846	0.08%	0.011%

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Sampling : 1

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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	13.603	2050	2053	2054	rVB2	805	497	0.05%	0.006%
78	13.628	2054	2057	2058	rBV2	642	577	0.06%	0.007%
79	13.689	2066	2067	2071	rBV4	481	677	0.07%	0.009%
80	13.780	2081	2082	2086	rBV3	1060	1161	0.11%	0.015%
81	13.938	2104	2108	2110	rBV2	539	620	0.06%	0.008%
82	14.024	2121	2122	2124	rBV2	529	480	0.05%	0.006%
83	14.127	2133	2139	2143	rBV3	1425	2868	0.28%	0.037%
84	14.335	2170	2173	2175	rVB2	659	619	0.06%	0.008%
85	14.451	2187	2192	2193	rBV2	1106	1168	0.12%	0.015%
86	14.585	2212	2214	2216	rBV2	678	509	0.05%	0.007%
87	14.658	2224	2226	2230	rVB3	707	621	0.06%	0.008%
88	14.701	2230	2233	2235	rBV2	571	638	0.06%	0.008%
89	14.719	2235	2236	2240	rVB3	628	560	0.06%	0.007%
90	14.896	2262	2265	2266	rBV3	826	635	0.06%	0.008%
91	15.054	2289	2291	2296	rVV3	806	904	0.09%	0.012%
92	15.389	2344	2346	2349	rVB3	1194	967	0.10%	0.012%
93	15.517	2365	2367	2369	rBV4	518	515	0.05%	0.007%
94	15.615	2381	2383	2384	rBV2	636	548	0.05%	0.007%
95	16.353	2502	2504	2505	rVB2	664	471	0.05%	0.006%
96	16.371	2505	2507	2509	rVB3	560	508	0.05%	0.007%
97	16.395	2509	2511	2513	rBV2	441	476	0.05%	0.006%
98	16.432	2516	2517	2521	rBV2	816	803	0.08%	0.010%
99	16.499	2527	2528	2530	rBV2	696	489	0.05%	0.006%
100	16.688	2556	2559	2560	rBV3	727	766	0.08%	0.010%

Sum of corrected areas: 7765767

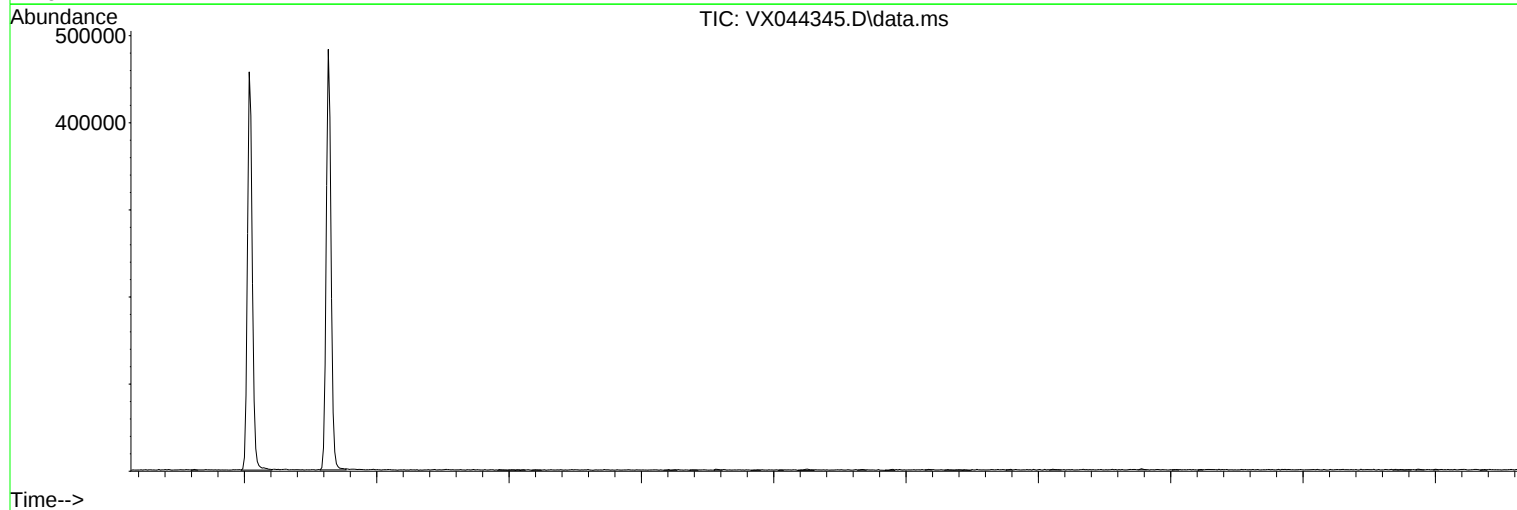
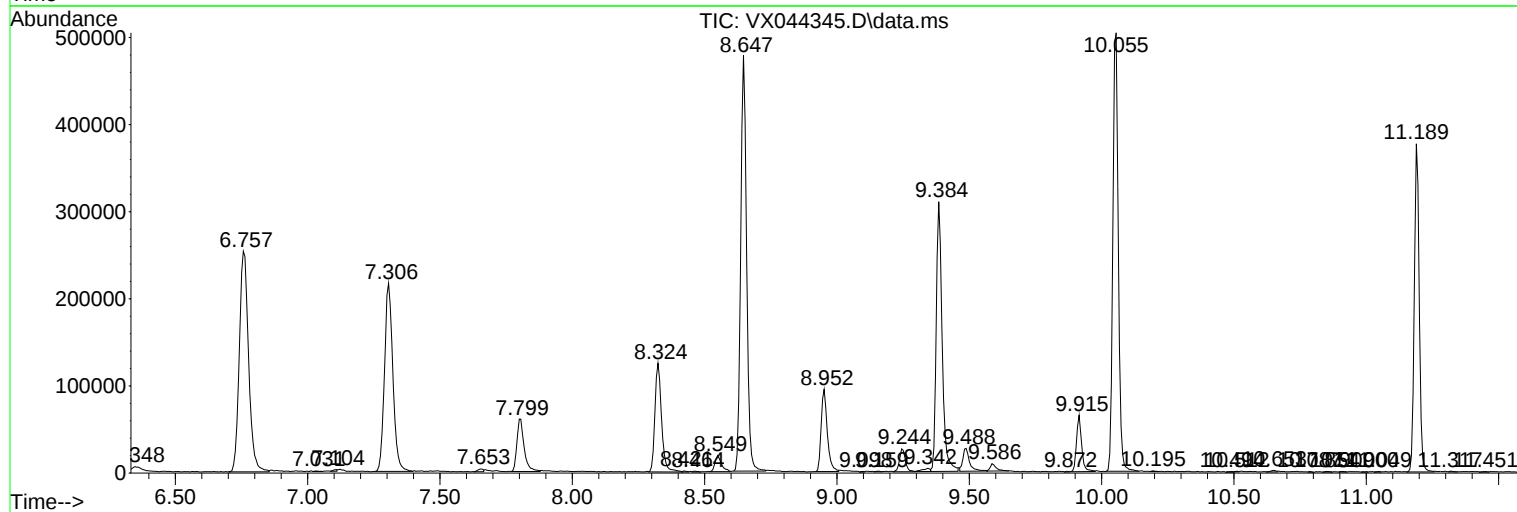
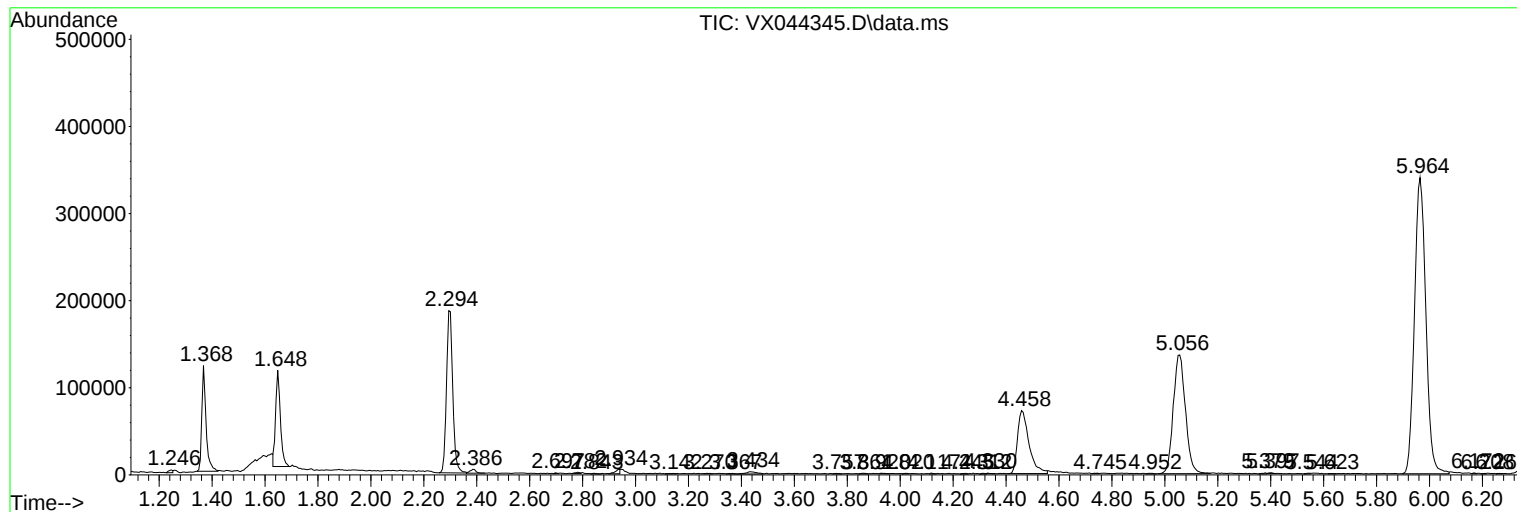
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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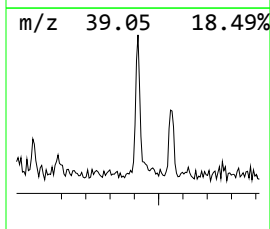
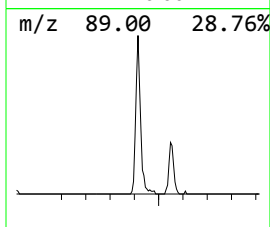
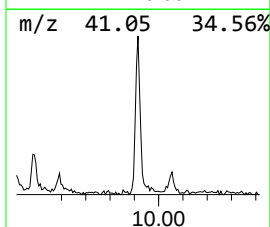
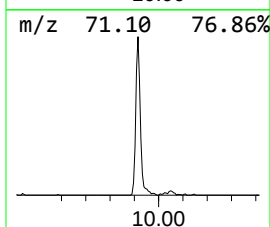
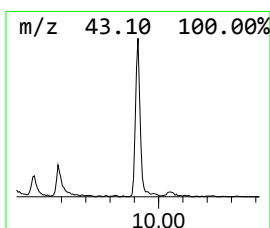
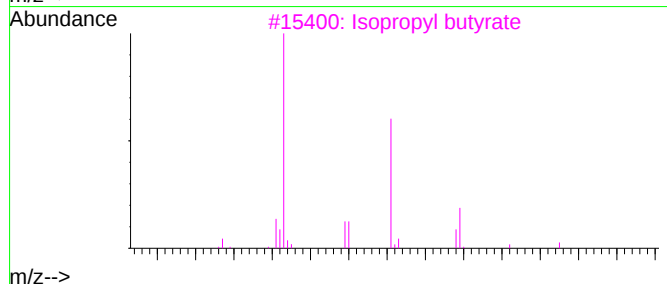
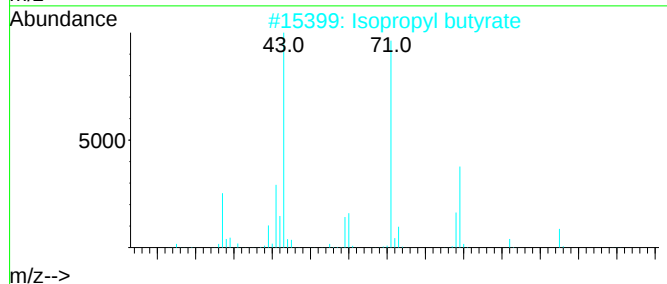
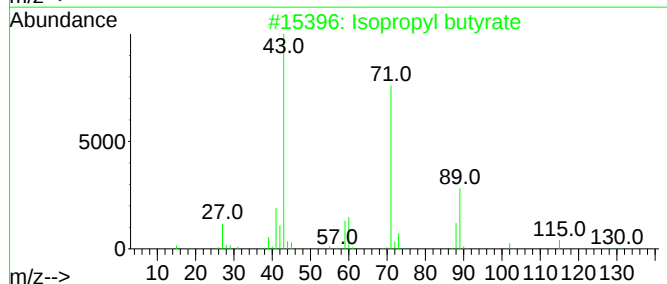
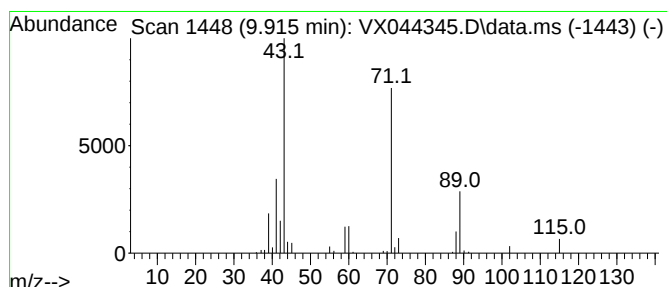
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	6.01 ug/L	86884	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	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl butyrate	9.915	6.0	ug/L	86884	2	10.055	722704	50.0