

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044339.D
 Acq On : 17 Dec 2024 10:26
 Operator : JC/MD
 Sample : P5235-07 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AT6

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: VX044339.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	26	rBV2	4688	3768	0.38%	0.049%
2	1.367	42	46	56	rBV	123520	131720	13.43%	1.725%
3	1.648	88	92	100	rVB	107673	151145	15.41%	1.979%
4	2.300	192	199	209	rBV	179730	294385	30.01%	3.854%
5	2.392	210	214	218	rVB3	3663	6292	0.64%	0.082%
6	2.501	230	232	235	rVB3	872	854	0.09%	0.011%
7	2.556	237	241	242	rBV4	683	738	0.08%	0.010%
8	2.636	252	254	257	rVB2	616	551	0.06%	0.007%
9	2.660	257	258	261	rBV3	568	530	0.05%	0.007%
10	2.794	274	280	285	rVB8	1594	3236	0.33%	0.042%
11	2.940	298	304	315	rVB	6134	13734	1.40%	0.180%
12	3.148	336	338	341	rVB3	638	581	0.06%	0.008%
13	3.428	377	384	385	rBV2	3087	4389	0.45%	0.057%
14	3.574	406	408	409	rBV2	809	794	0.08%	0.010%
15	3.672	421	424	426	rBV3	615	683	0.07%	0.009%
16	3.721	430	432	435	rBV3	848	725	0.07%	0.009%
17	3.794	440	444	447	rBV4	622	896	0.09%	0.012%
18	4.068	487	489	492	rVB3	756	697	0.07%	0.009%
19	4.233	514	516	519	rBV4	559	555	0.06%	0.007%
20	4.263	519	521	522	rBV2	549	518	0.05%	0.007%
21	4.458	546	553	567	rBV	66052	200528	20.44%	2.626%
22	4.940	630	632	636	rVB2	769	893	0.09%	0.012%
23	4.970	636	637	639	rBV2	885	791	0.08%	0.010%
24	5.050	640	650	665	rVV	133350	413403	42.14%	5.413%
25	5.300	689	691	694	rVB2	724	660	0.07%	0.009%
26	5.385	702	705	706	rBV3	955	717	0.07%	0.009%
27	5.428	710	712	716	rBV3	684	997	0.10%	0.013%
28	5.537	726	730	731	rBV3	955	1241	0.13%	0.016%
29	5.684	752	754	758	rBV3	655	671	0.07%	0.009%
30	5.800	772	773	776	rVB2	664	602	0.06%	0.008%
31	5.964	788	800	823	rBV3	326759	981113	100.00%	12.846%
32	6.354	857	864	871	rBV3	6568	18046	1.84%	0.236%
33	6.671	913	916	919	rBV3	540	674	0.07%	0.009%
34	6.757	921	930	945	rBV	258273	617809	62.97%	8.089%
35	7.043	975	977	979	rBV3	465	531	0.05%	0.007%
36	7.110	983	988	990	rBV4	2782	4185	0.43%	0.055%

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 Title : VOC Analysis

37	7.159	995	996	999	rVB3	685	560	0.06%	0.007%
38	7.305	1012	1020	1031	rBV	205437	451078	45.98%	5.906%
39	7.568	1060	1063	1064	rBV4	483	580	0.06%	0.008%
40	7.665	1073	1079	1081	rBV5	2697	5294	0.54%	0.069%
41	7.799	1096	1101	1111	rBV	86664	159975	16.31%	2.095%
42	8.324	1181	1187	1201	rBV	120981	209307	21.33%	2.740%
43	8.549	1219	1224	1233	rBV	18949	36371	3.71%	0.476%
44	8.647	1233	1240	1254	rVV	462248	716632	73.04%	9.383%
45	8.891	1278	1280	1284	rVB4	596	716	0.07%	0.009%
46	8.951	1284	1290	1298	rBV2	107068	170318	17.36%	2.230%
47	9.244	1331	1338	1345	rBV	28732	42514	4.33%	0.557%
48	9.384	1356	1361	1373	rBV	290710	440839	44.93%	5.772%
49	9.488	1374	1378	1389	rVB	38746	58652	5.98%	0.768%
50	9.579	1390	1393	1402	rVB	19406	30188	3.08%	0.395%
51	9.915	1443	1448	1456	rBV	75753	102577	10.46%	1.343%
52	10.055	1465	1471	1486	rVB	512036	720581	73.45%	9.435%
53	10.268	1505	1506	1509	rBV3	745	523	0.05%	0.007%
54	10.293	1509	1510	1517	rVV5	859	1473	0.15%	0.019%
55	10.348	1517	1519	1521	rVB3	1081	774	0.08%	0.010%
56	10.439	1531	1534	1535	rBV2	713	645	0.07%	0.008%
57	10.518	1545	1547	1550	rBV2	919	774	0.08%	0.010%
58	10.646	1565	1568	1572	rBV4	3000	4356	0.44%	0.057%
59	11.091	1638	1641	1643	rBV2	384	541	0.06%	0.007%
60	11.189	1652	1657	1667	rBV	366029	457224	46.60%	5.986%
61	11.402	1690	1692	1694	rVV2	782	614	0.06%	0.008%
62	11.512	1708	1710	1713	rBV	842	845	0.09%	0.011%
63	11.591	1721	1723	1727	rBV4	477	738	0.08%	0.010%
64	11.664	1732	1735	1736	rBV3	806	817	0.08%	0.011%
65	11.805	1755	1758	1760	rBV2	835	771	0.08%	0.010%
66	11.884	1769	1771	1774	rBV3	444	520	0.05%	0.007%
67	11.945	1777	1781	1782	rBV3	678	800	0.08%	0.010%
68	12.018	1788	1793	1803	rBV	430548	565429	57.63%	7.403%
69	12.317	1837	1842	1853	rBV	449333	571697	58.27%	7.485%
70	12.762	1913	1915	1920	rVB2	1149	1288	0.13%	0.017%
71	12.811	1920	1923	1925	rBV2	507	615	0.06%	0.008%
72	12.926	1941	1942	1945	rVB3	890	666	0.07%	0.009%
73	13.012	1954	1956	1961	rBV3	418	709	0.07%	0.009%
74	13.091	1963	1969	1972	rVB3	530	981	0.10%	0.013%
75	13.359	2010	2013	2015	rBV	540	582	0.06%	0.008%
76	13.420	2019	2023	2026	rBV5	636	724	0.07%	0.009%

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Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

77	13.640	2055	2059	2060	rBV	1009	896	0.09%	0.012%
78	13.719	2069	2072	2073	rBV2	646	738	0.08%	0.010%
79	13.920	2104	2105	2107	rBV2	674	634	0.06%	0.008%
80	14.127	2135	2139	2143	rVV3	1202	1875	0.19%	0.025%
81	14.182	2143	2148	2151	rVV3	717	1134	0.12%	0.015%
82	14.341	2173	2174	2177	rBV2	913	980	0.10%	0.013%
83	14.426	2186	2188	2190	rBV3	671	613	0.06%	0.008%
84	14.451	2190	2192	2195	rBV3	819	786	0.08%	0.010%
85	14.676	2228	2229	2232	rVB3	653	529	0.05%	0.007%
86	14.700	2232	2233	2236	rBV3	513	544	0.06%	0.007%
87	14.847	2253	2257	2258	rBV2	614	587	0.06%	0.008%
88	15.213	2315	2317	2319	rBV	681	643	0.07%	0.008%
89	15.237	2319	2321	2323	rVB3	761	670	0.07%	0.009%
90	15.274	2325	2327	2331	rVB2	931	923	0.09%	0.012%
91	15.560	2373	2374	2377	rBV2	601	620	0.06%	0.008%
92	15.792	2410	2412	2414	rVB2	786	616	0.06%	0.008%
93	15.956	2437	2439	2443	rVB3	609	537	0.05%	0.007%
94	16.212	2477	2481	2482	rBV2	915	664	0.07%	0.009%
95	16.438	2516	2518	2519	rBV	1143	593	0.06%	0.008%
96	16.475	2522	2524	2527	rVB3	735	556	0.06%	0.007%
97	16.505	2527	2529	2531	rBV2	863	636	0.06%	0.008%
98	16.645	2550	2552	2554	rBV2	795	554	0.06%	0.007%
99	16.706	2560	2562	2563	rBV2	628	512	0.05%	0.007%
100	16.724	2563	2565	2569	rVB4	748	859	0.09%	0.011%

Sum of corrected areas: 7637639

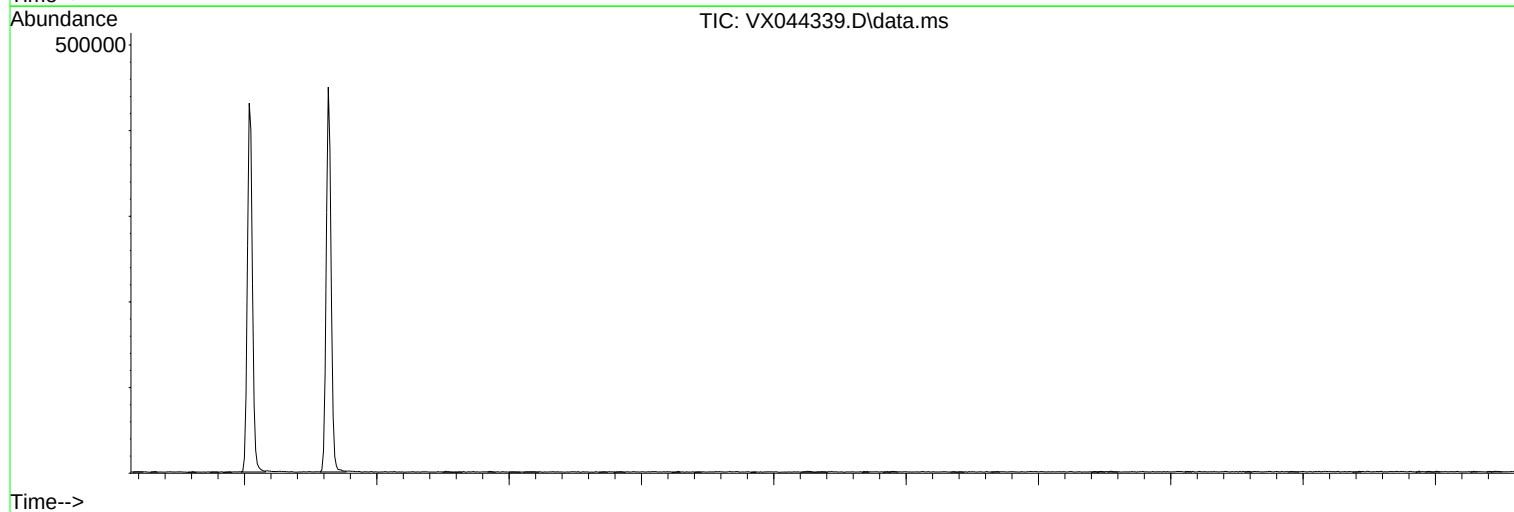
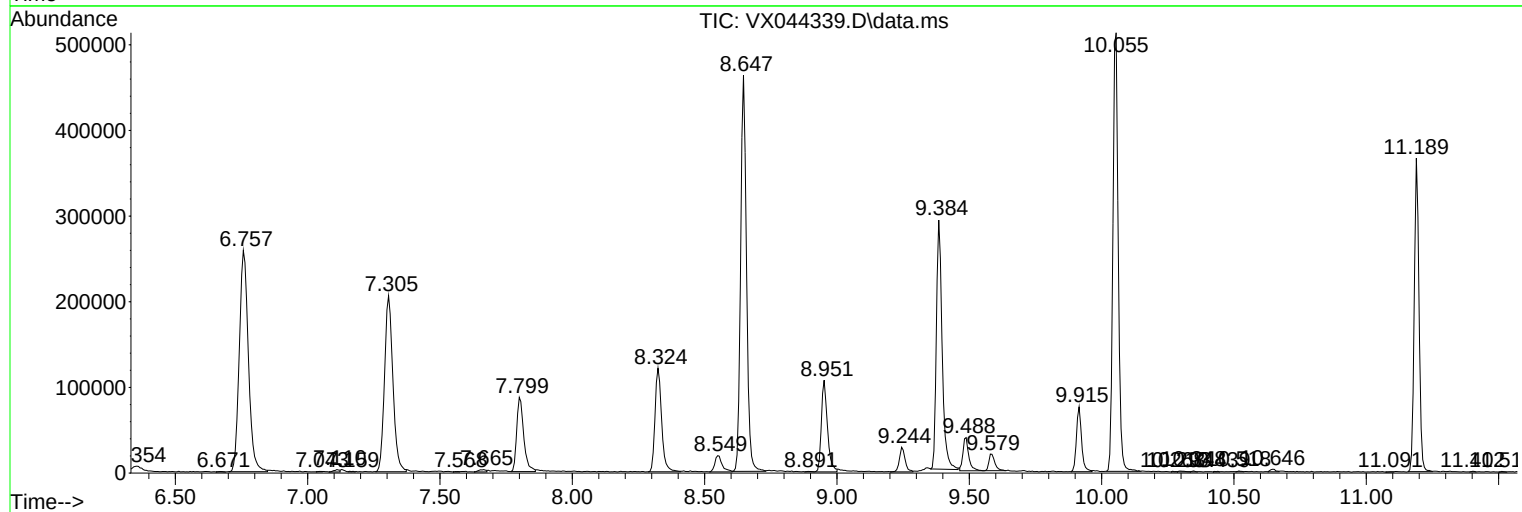
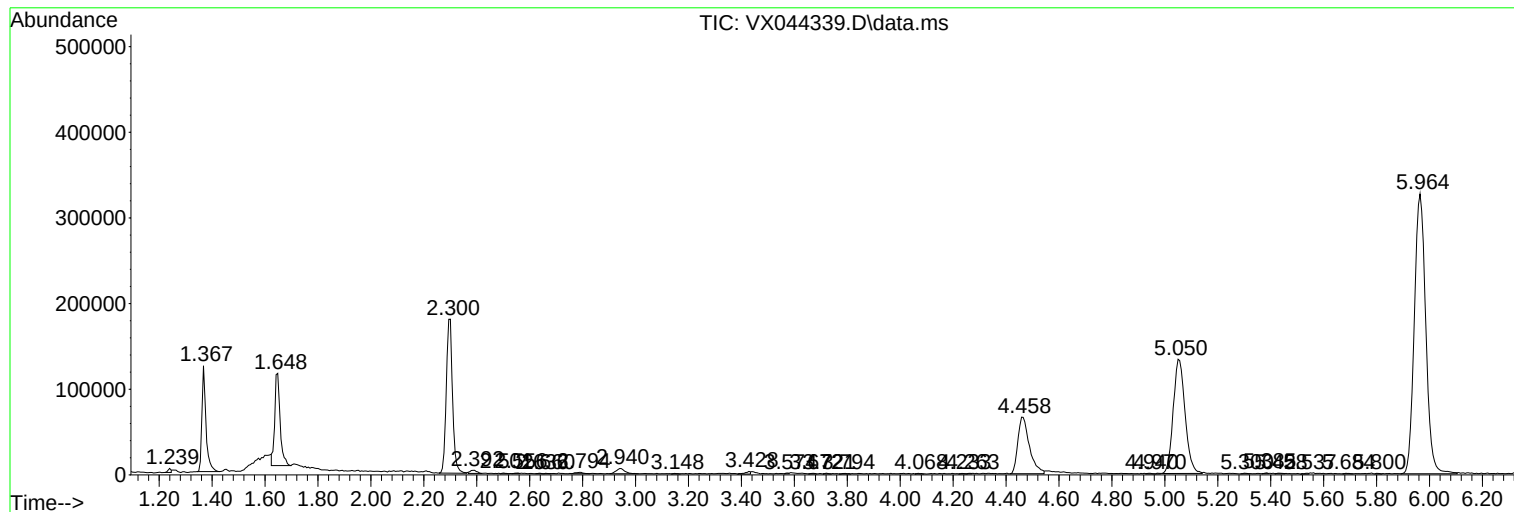
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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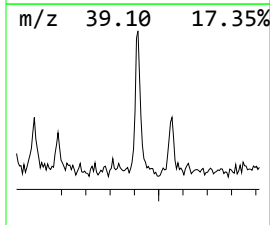
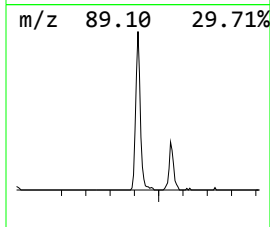
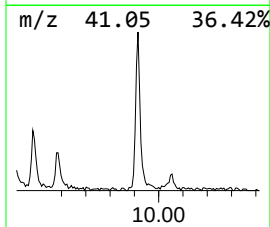
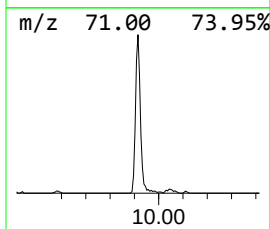
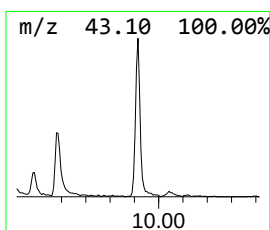
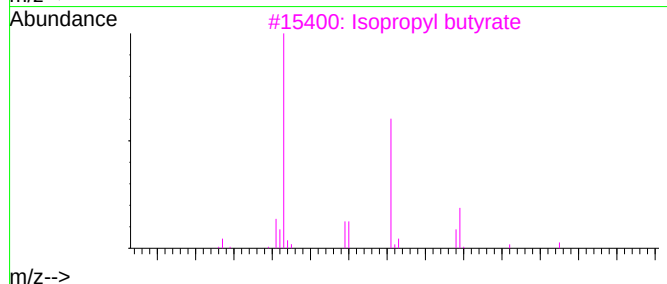
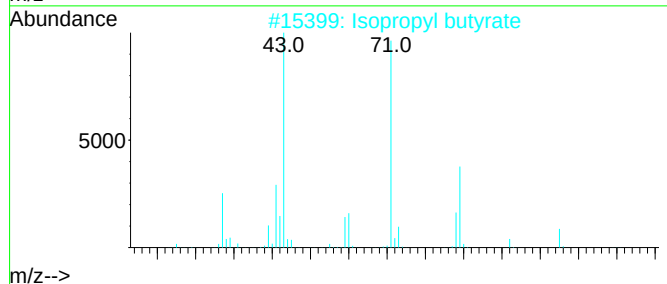
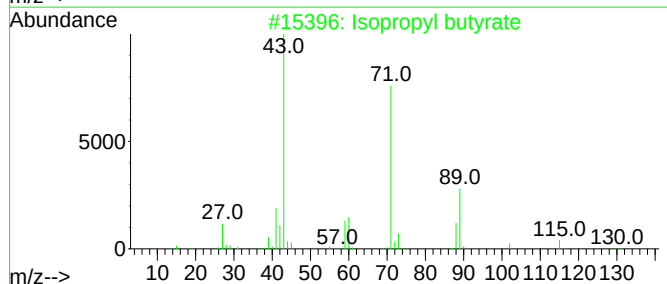
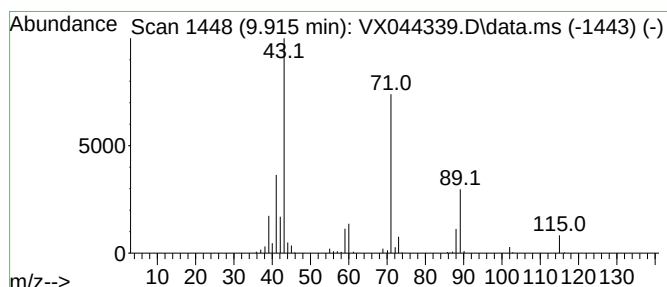
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	7.12 ug/L	102577	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	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



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TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isopropyl butyrate	9.915	7.1	ug/L	102577	2	10.055	720581	50.0