

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044343.D
 Acq On : 17 Dec 2024 11:58
 Operator : JC/MD
 Sample : P5235-02 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COATO

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: VX044343.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	23	25	27	rBV	4458	4416	0.44%	0.057%
2	1.368	42	46	54	rBV	122400	134188	13.40%	1.746%
3	1.642	88	91	107	rVB	118047	175969	17.57%	2.290%
4	2.294	192	198	208	rVV	192403	299224	29.88%	3.894%
5	2.386	209	213	221	rVB	5967	11017	1.10%	0.143%
6	2.697	262	264	266	rBV3	841	1001	0.10%	0.013%
7	2.782	275	278	281	rBV4	1254	1946	0.19%	0.025%
8	2.825	283	285	288	rBV2	592	656	0.07%	0.009%
9	2.941	297	304	312	rBV2	6832	15671	1.56%	0.204%
10	3.099	328	330	331	rBV2	557	476	0.05%	0.006%
11	3.343	364	370	371	rBV3	1070	1469	0.15%	0.019%
12	3.434	380	385	388	rVV3	2415	4466	0.45%	0.058%
13	3.477	391	392	395	rVB2	848	518	0.05%	0.007%
14	3.544	401	403	406	rBV2	464	623	0.06%	0.008%
15	3.581	406	409	411	rBV3	1152	1341	0.13%	0.017%
16	3.648	419	420	423	rBV2	560	485	0.05%	0.006%
17	3.751	435	437	439	rVB2	625	399	0.04%	0.005%
18	3.782	439	442	445	rBV3	651	868	0.09%	0.011%
19	3.977	472	474	477	rBV3	587	457	0.05%	0.006%
20	4.172	505	506	508	rVV	666	407	0.04%	0.005%
21	4.196	508	510	511	rVV	528	396	0.04%	0.005%
22	4.227	513	515	516	rVB2	662	429	0.04%	0.006%
23	4.379	539	540	542	rVB	731	441	0.04%	0.006%
24	4.410	542	545	546	rBV2	514	518	0.05%	0.007%
25	4.465	546	554	569	rBV	69586	210674	21.04%	2.742%
26	4.702	591	593	595	rBV2	789	564	0.06%	0.007%
27	5.056	639	651	668	rBV2	138032	424380	42.38%	5.523%
28	5.233	678	680	686	rVB4	784	894	0.09%	0.012%
29	5.361	699	701	702	rBV	843	558	0.06%	0.007%
30	5.391	704	706	707	rBV2	616	425	0.04%	0.006%
31	5.519	725	727	729	rBV3	473	435	0.04%	0.006%
32	5.647	745	748	749	rBV3	668	430	0.04%	0.006%
33	5.660	749	750	752	rBV2	553	485	0.05%	0.006%
34	5.794	770	772	774	rBV	546	479	0.05%	0.006%
35	5.873	783	785	788	rBV3	432	427	0.04%	0.006%
36	5.964	788	800	821	rBV2	339439	1001397	100.00%	13.033%

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 Title : VOC Analysis

37	6.196	837	838	842	rVV2	664	659	0.07%	0.009%
38	6.239	842	845	847	rVV3	905	597	0.06%	0.008%
39	6.355	857	864	873	rBV2	6039	15422	1.54%	0.201%
40	6.574	896	900	901	rVB3	594	514	0.05%	0.007%
41	6.757	921	930	947	rBV	255537	624710	62.38%	8.131%
42	7.306	1012	1020	1032	rBV	211390	466554	46.59%	6.072%
43	7.592	1065	1067	1068	rBV2	610	466	0.05%	0.006%
44	7.659	1073	1078	1082	rBV3	2949	5994	0.60%	0.078%
45	7.799	1096	1101	1114	rBV	55848	108598	10.84%	1.413%
46	7.940	1122	1124	1126	rVB2	717	501	0.05%	0.007%
47	8.196	1164	1166	1170	rBV3	675	567	0.06%	0.007%
48	8.324	1181	1187	1196	rBV	124692	209267	20.90%	2.724%
49	8.549	1219	1224	1233	rBV2	16988	29974	2.99%	0.390%
50	8.647	1234	1240	1253	rBV	470847	732211	73.12%	9.530%
51	8.793	1262	1264	1267	rVB3	928	893	0.09%	0.012%
52	8.952	1284	1290	1300	rBV2	91853	147692	14.75%	1.922%
53	9.244	1333	1338	1347	rBV	24820	39179	3.91%	0.510%
54	9.342	1352	1354	1356	rVV3	4126	4345	0.43%	0.057%
55	9.384	1356	1361	1374	rVV	305965	462274	46.16%	6.016%
56	9.488	1374	1378	1384	rVB	31514	45026	4.50%	0.586%
57	9.586	1390	1394	1404	rVB3	11332	19135	1.91%	0.249%
58	9.695	1411	1412	1414	rBV2	813	554	0.06%	0.007%
59	9.915	1442	1448	1459	rBV	69354	97915	9.78%	1.274%
60	10.055	1465	1471	1484	rBV	498707	720099	71.91%	9.372%
61	10.262	1503	1505	1506	rBV2	794	727	0.07%	0.009%
62	10.451	1534	1536	1539	rVB2	651	568	0.06%	0.007%
63	10.518	1545	1547	1549	rBV2	911	771	0.08%	0.010%
64	10.573	1555	1556	1559	rBV2	577	521	0.05%	0.007%
65	10.653	1565	1569	1572	rBV4	3052	4803	0.48%	0.063%
66	11.091	1636	1641	1642	rBV4	635	943	0.09%	0.012%
67	11.189	1652	1657	1666	rBV	358416	469460	46.88%	6.110%
68	11.463	1698	1702	1705	rBV3	704	1000	0.10%	0.013%
69	11.610	1724	1726	1729	rBV2	657	663	0.07%	0.009%
70	11.640	1729	1731	1733	rVB2	504	403	0.04%	0.005%
71	11.835	1761	1763	1766	rBV2	407	436	0.04%	0.006%
72	12.018	1788	1793	1803	rBV	439577	564858	56.41%	7.352%
73	12.317	1837	1842	1853	rBV	454423	589549	58.87%	7.673%
74	12.573	1883	1884	1887	rBV3	439	408	0.04%	0.005%
75	12.616	1890	1891	1895	rBV3	496	468	0.05%	0.006%
76	12.701	1900	1905	1907	rVB4	854	1436	0.14%	0.019%

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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\SFAMXLM120524WMA.M
 Title : VOC Analysis

77	12.719	1907	1908	1910	rBV	856	810	0.08%	0.011%
78	12.872	1931	1933	1936	rVB2	960	843	0.08%	0.011%
79	12.896	1936	1937	1940	rBV2	641	441	0.04%	0.006%
80	12.927	1940	1942	1944	rBV2	616	677	0.07%	0.009%
81	12.987	1948	1952	1955	rVB3	971	1204	0.12%	0.016%
82	13.030	1957	1959	1962	rBV4	483	564	0.06%	0.007%
83	13.317	2004	2006	2007	rBV2	622	629	0.06%	0.008%
84	13.579	2047	2049	2050	rBV	721	570	0.06%	0.007%
85	13.628	2056	2057	2060	rVV2	603	627	0.06%	0.008%
86	13.780	2080	2082	2083	rBV2	658	490	0.05%	0.006%
87	13.963	2111	2112	2115	rBV3	609	648	0.06%	0.008%
88	14.024	2120	2122	2125	rVB3	434	472	0.05%	0.006%
89	14.499	2197	2200	2201	rBV2	708	747	0.07%	0.010%
90	14.548	2206	2208	2210	rBV2	738	517	0.05%	0.007%
91	14.664	2225	2227	2228	rVB	837	401	0.04%	0.005%
92	14.957	2273	2275	2277	rVB2	898	579	0.06%	0.008%
93	14.993	2277	2281	2282	rBV3	759	1022	0.10%	0.013%
94	15.103	2297	2299	2301	rBV2	514	552	0.06%	0.007%
95	15.329	2335	2336	2338	rBV2	659	526	0.05%	0.007%
96	15.481	2359	2361	2362	rBV2	566	463	0.05%	0.006%
97	15.761	2405	2407	2410	rBV3	694	502	0.05%	0.007%
98	15.993	2444	2445	2448	rVB2	877	553	0.06%	0.007%
99	16.408	2511	2513	2514	rBV2	577	502	0.05%	0.007%
100	16.706	2560	2562	2564	rBV2	646	477	0.05%	0.006%

Sum of corrected areas: 7683505

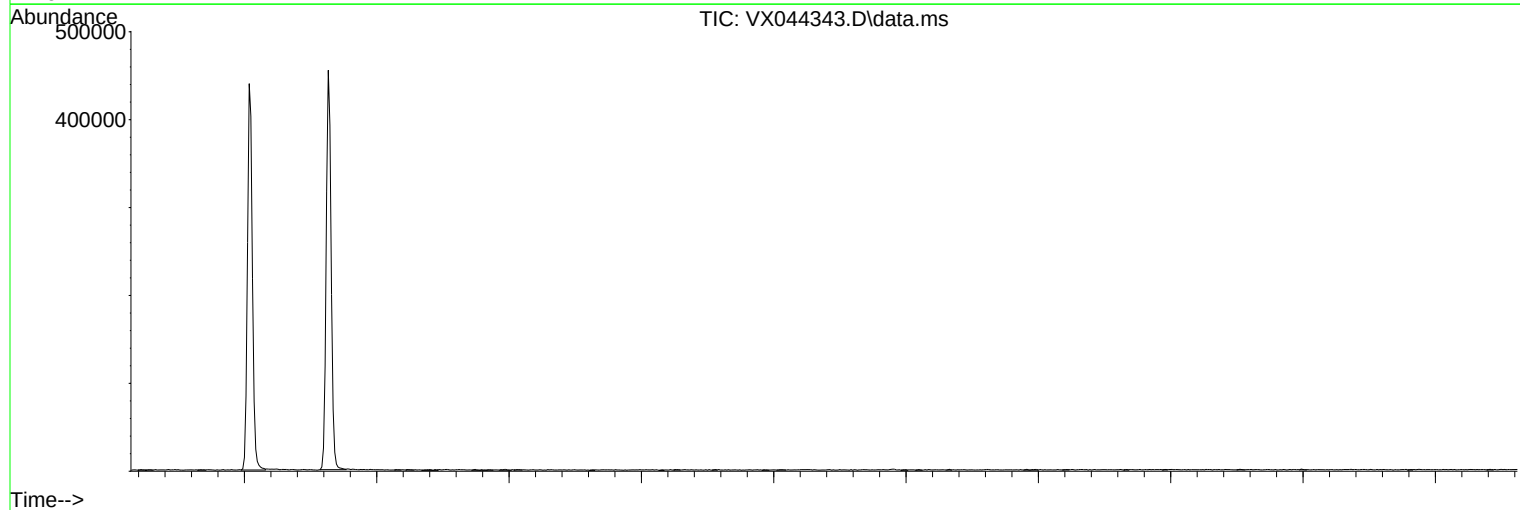
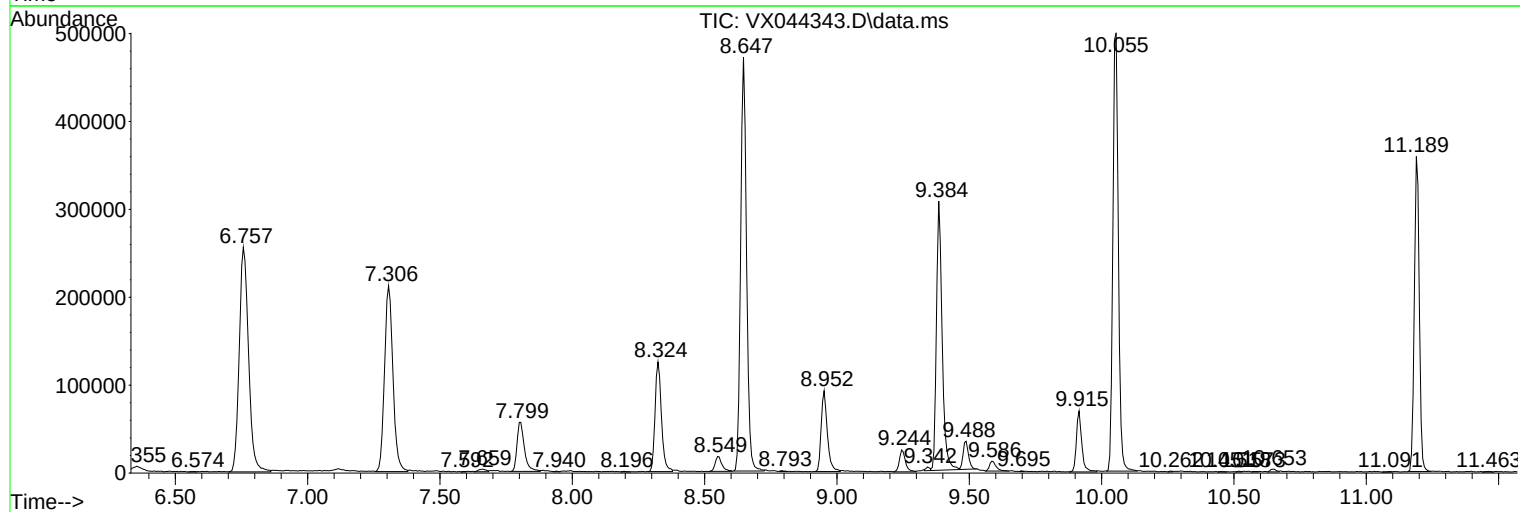
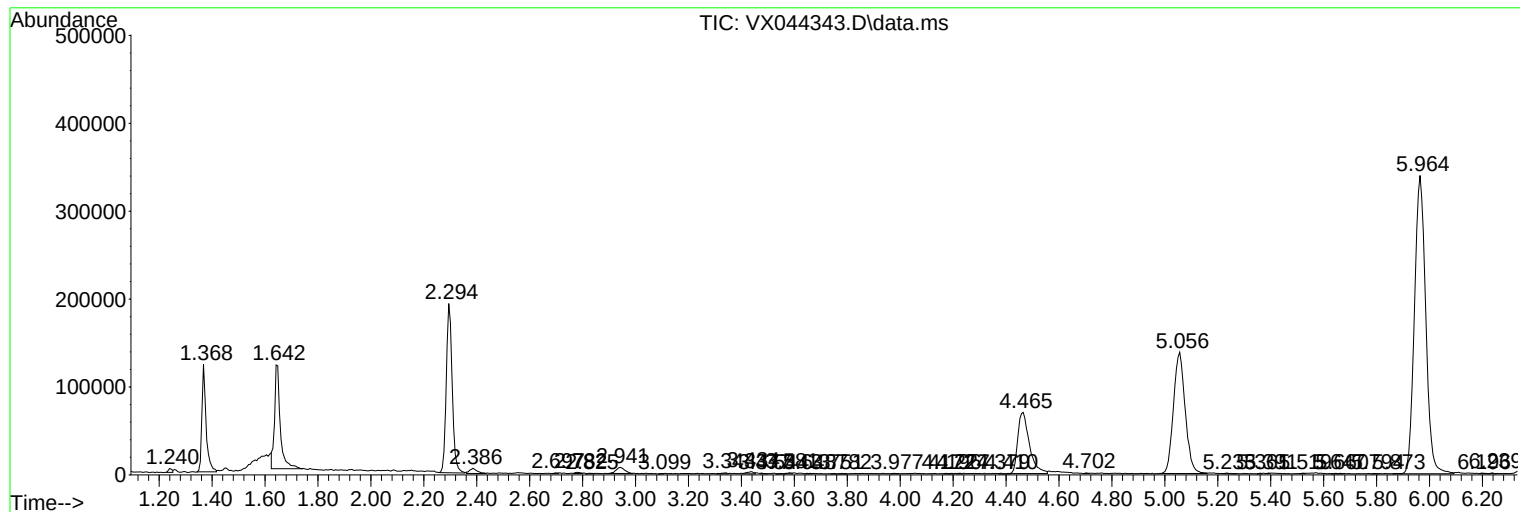
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COAT0

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

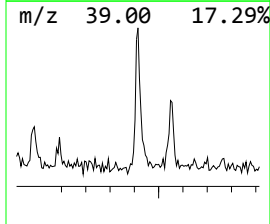
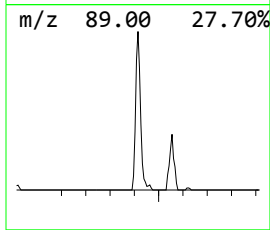
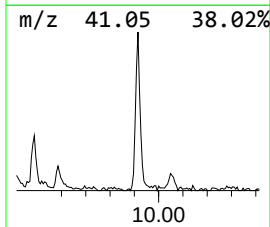
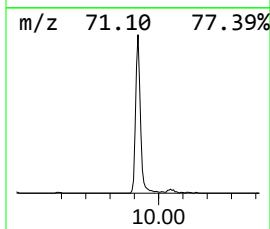
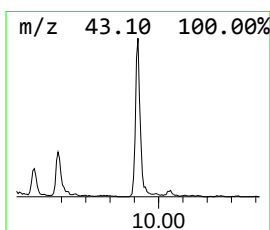
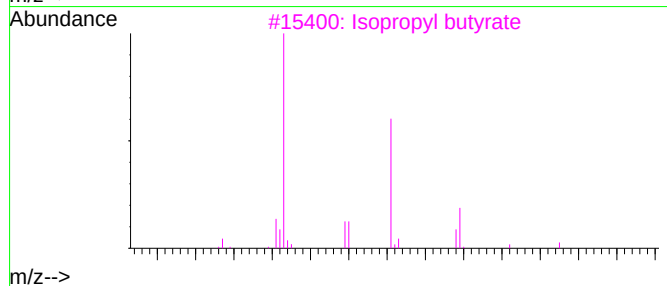
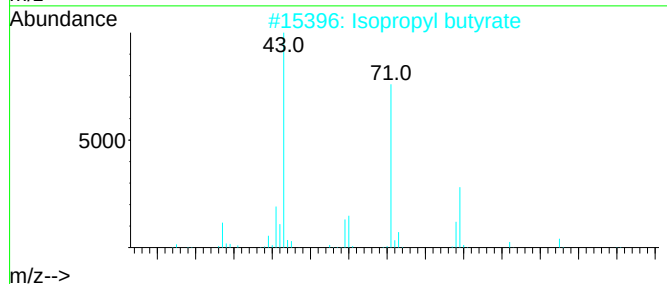
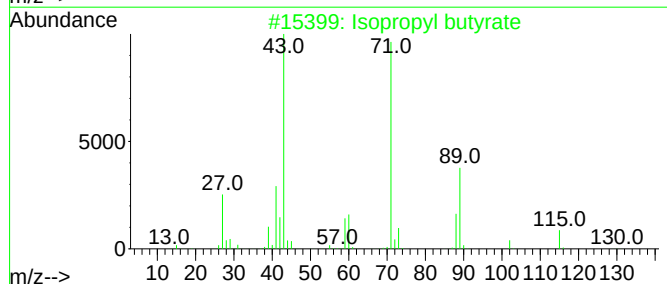
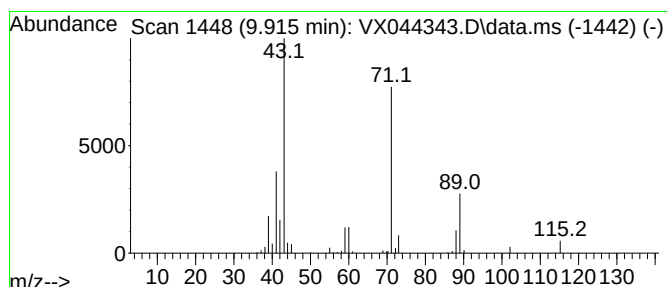
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	6.80 ug/L	97915	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	56
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	50



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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	#	RT	Resp	Conc
Isopropyl butyrate	9.915	6.8	ug/L	97915	2	10.055	720099	50.0