

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044342.D
 Acq On : 17 Dec 2024 11:35
 Operator : JC/MD
 Sample : P5235-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AS8

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: VX044342.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	32	rVB2	6806	11332	1.15%	0.148%
2	1.367	42	46	55	rBV	114739	127791	12.93%	1.666%
3	1.648	88	92	100	rVB	106164	145012	14.67%	1.890%
4	2.294	192	198	209	rBV	190856	298091	30.15%	3.886%
5	2.392	210	214	220	rVB	4689	8083	0.82%	0.105%
6	2.636	253	254	257	rBV2	764	605	0.06%	0.008%
7	2.666	257	259	261	rBV	725	808	0.08%	0.011%
8	2.703	263	265	266	rBV2	869	848	0.09%	0.011%
9	2.782	274	278	279	rBV3	1354	1746	0.18%	0.023%
10	2.837	286	287	291	rVB3	584	694	0.07%	0.009%
11	2.867	291	292	295	rBV2	499	575	0.06%	0.007%
12	2.946	298	305	312	rVB2	6319	14537	1.47%	0.190%
13	3.306	362	364	367	rBV2	404	489	0.05%	0.006%
14	3.343	367	370	374	rBV4	774	1512	0.15%	0.020%
15	3.434	380	385	386	rBV3	1866	2909	0.29%	0.038%
16	3.587	403	410	414	rBV4	1196	2386	0.24%	0.031%
17	3.770	438	440	441	rBV	836	589	0.06%	0.008%
18	3.794	441	444	446	rBV3	689	738	0.07%	0.010%
19	4.038	481	484	486	rBV2	612	663	0.07%	0.009%
20	4.245	514	518	519	rBV3	354	448	0.05%	0.006%
21	4.276	519	523	526	rBV3	579	689	0.07%	0.009%
22	4.458	546	553	567	rBV	70716	204692	20.70%	2.668%
23	4.733	596	598	600	rBV2	932	789	0.08%	0.010%
24	5.056	639	651	671	rBV2	134551	421950	42.68%	5.500%
25	5.367	698	702	703	rVB3	478	523	0.05%	0.007%
26	5.385	703	705	709	rBV3	1011	1289	0.13%	0.017%
27	5.708	756	758	759	rBV2	616	491	0.05%	0.006%
28	5.787	769	771	775	rVV3	444	506	0.05%	0.007%
29	5.964	789	800	820	rBV2	333625	988685	100.00%	12.888%
30	6.281	848	852	854	rBV4	515	529	0.05%	0.007%
31	6.348	856	863	875	rVV3	6420	19491	1.97%	0.254%
32	6.757	921	930	943	rBV	247052	593921	60.07%	7.742%
33	7.305	1011	1020	1042	rBV	207419	461684	46.70%	6.018%
34	7.659	1073	1078	1083	rBV2	3315	7085	0.72%	0.092%
35	7.799	1095	1101	1114	rBV	86524	163301	16.52%	2.129%
36	8.153	1157	1159	1162	rBV	484	658	0.07%	0.009%

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

37	8.238	1170	1173	1174	rVB3	616	541	0.05%	0.007%
38	8.257	1174	1176	1177	rBV2	698	500	0.05%	0.007%
39	8.324	1181	1187	1201	rVV	127946	211796	21.42%	2.761%
40	8.549	1219	1224	1234	rBV	19779	33841	3.42%	0.441%
41	8.647	1234	1240	1255	rVV	465617	726793	73.51%	9.474%
42	8.952	1284	1290	1306	rBV2	101937	170236	17.22%	2.219%
43	9.201	1329	1331	1333	rBV2	643	497	0.05%	0.006%
44	9.244	1333	1338	1346	rVV	28167	42260	4.27%	0.551%
45	9.384	1356	1361	1373	rVV	311590	452567	45.77%	5.900%
46	9.488	1374	1378	1389	rVB	38616	59414	6.01%	0.775%
47	9.586	1390	1394	1403	rVB	21680	30964	3.13%	0.404%
48	9.750	1419	1421	1425	rVB2	519	645	0.07%	0.008%
49	9.823	1432	1433	1435	rBV	519	437	0.04%	0.006%
50	9.854	1436	1438	1439	rVB2	893	442	0.04%	0.006%
51	9.915	1443	1448	1457	rVV	73333	101469	10.26%	1.323%
52	10.055	1465	1471	1483	rBV	497262	706954	71.50%	9.216%
53	10.201	1494	1495	1496	rVB	1182	433	0.04%	0.006%
54	10.232	1498	1500	1502	rBV2	783	590	0.06%	0.008%
55	10.421	1528	1531	1535	rVB4	747	1253	0.13%	0.016%
56	10.476	1538	1540	1542	rBV2	640	642	0.06%	0.008%
57	10.518	1543	1547	1548	rBV3	517	687	0.07%	0.009%
58	10.646	1565	1568	1572	rBV6	2952	4676	0.47%	0.061%
59	10.762	1584	1587	1589	rBV3	613	853	0.09%	0.011%
60	11.189	1652	1657	1672	rVB	362600	474825	48.03%	6.190%
61	11.457	1700	1701	1704	rVV3	739	748	0.08%	0.010%
62	11.512	1708	1710	1713	rVB3	566	583	0.06%	0.008%
63	11.561	1716	1718	1722	rVB3	527	615	0.06%	0.008%
64	11.603	1722	1725	1728	rBB3	775	744	0.08%	0.010%
65	11.628	1728	1729	1733	rBV3	554	567	0.06%	0.007%
66	11.658	1733	1734	1737	rBV3	681	466	0.05%	0.006%
67	11.689	1737	1739	1742	rVV2	420	530	0.05%	0.007%
68	11.762	1748	1751	1756	rVV4	657	945	0.10%	0.012%
69	12.018	1788	1793	1803	rBV	430354	553565	55.99%	7.216%
70	12.317	1837	1842	1849	rBV	449369	584005	59.07%	7.613%
71	12.701	1903	1905	1908	rBV3	478	614	0.06%	0.008%
72	12.798	1919	1921	1924	rVB3	538	507	0.05%	0.007%
73	13.018	1955	1957	1960	rBV3	865	852	0.09%	0.011%
74	13.054	1960	1963	1964	rBV2	552	548	0.06%	0.007%
75	13.213	1988	1989	1992	rVB2	562	462	0.05%	0.006%
76	13.780	2080	2082	2085	rBV2	418	477	0.05%	0.006%

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 Title : VOC Analysis

77	13.829	2089	2090	2092	rBV	632	443	0.04%	0.006%
78	13.908	2102	2103	2106	rBV2	432	505	0.05%	0.007%
79	14.054	2124	2127	2128	rBV3	547	660	0.07%	0.009%
80	14.103	2131	2135	2136	rBV3	396	491	0.05%	0.006%
81	14.121	2136	2138	2139	rBV	864	539	0.05%	0.007%
82	14.182	2146	2148	2150	rVB2	703	441	0.04%	0.006%
83	14.249	2157	2159	2161	rVB3	557	564	0.06%	0.007%
84	14.511	2199	2202	2203	rBV2	430	578	0.06%	0.008%
85	14.780	2243	2246	2250	rBV3	831	1270	0.13%	0.017%
86	14.932	2270	2271	2275	rBV3	664	741	0.07%	0.010%
87	14.969	2275	2277	2279	rBV2	726	558	0.06%	0.007%
88	15.097	2296	2298	2304	rBV5	459	988	0.10%	0.013%
89	15.237	2320	2321	2323	rBV	795	617	0.06%	0.008%
90	15.670	2390	2392	2393	rBV2	671	455	0.05%	0.006%
91	15.688	2393	2395	2398	rVB2	720	651	0.07%	0.008%
92	15.719	2398	2400	2401	rBV2	601	468	0.05%	0.006%
93	15.895	2427	2429	2433	rVV3	710	809	0.08%	0.011%
94	15.999	2445	2446	2449	rVB2	837	590	0.06%	0.008%
95	16.115	2463	2465	2467	rBV	721	678	0.07%	0.009%
96	16.182	2472	2476	2478	rBV4	844	846	0.09%	0.011%
97	16.444	2517	2519	2522	rVB3	617	694	0.07%	0.009%
98	16.615	2545	2547	2550	rBV2	602	617	0.06%	0.008%
99	16.645	2550	2552	2554	rVB2	580	592	0.06%	0.008%
100	16.676	2554	2557	2558	rBV2	820	719	0.07%	0.009%

Sum of corrected areas: 7671196

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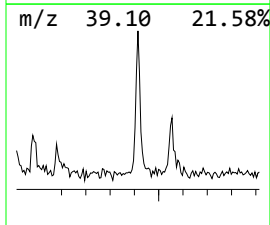
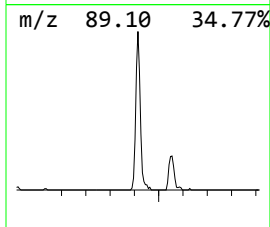
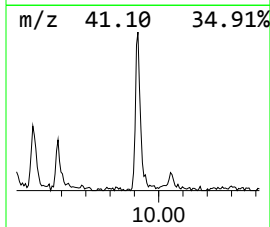
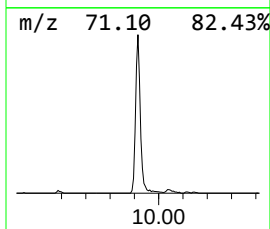
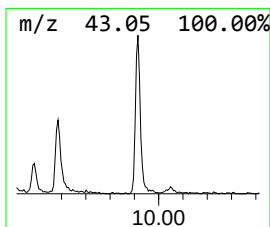
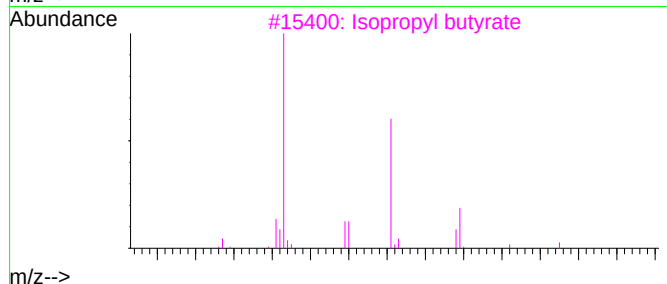
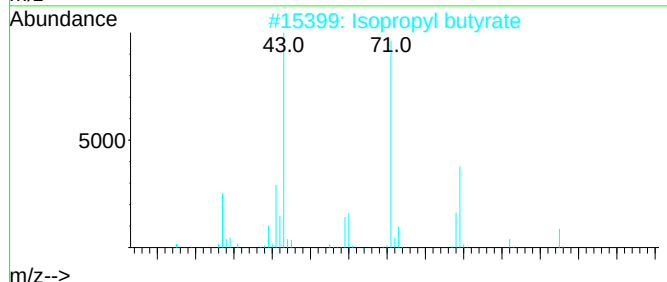
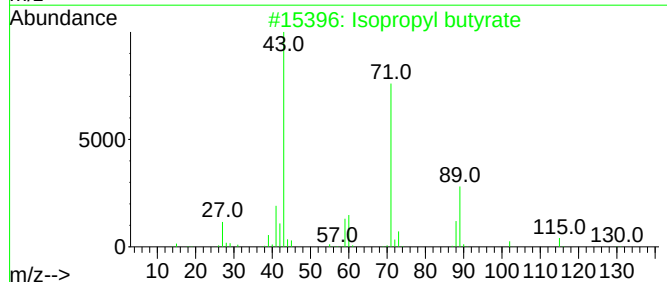
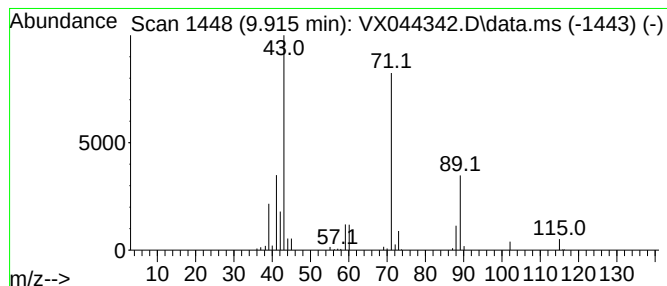
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

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	7.18 ug/L	101469	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	83
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	78
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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TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isopropyl butyrate	9.915	7.2	ug/L	101469	2	10.055	706954	50.0