

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044349.D
 Acq On : 17 Dec 2024 14:18
 Operator : JC/MD
 Sample : P5235-10 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AW0

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\SFAMXML120524WMA.M
 Title : VOC Analysis

Signal : TIC: VX044349.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	12	rVB2	1661	1167	0.12%	0.015%
2	1.240	23	25	26	rBV2	2955	2255	0.22%	0.030%
3	1.368	42	46	57	rBV	119758	130500	12.99%	1.710%
4	1.648	89	92	100	rVB	114874	144573	14.39%	1.895%
5	2.294	192	198	208	rBV	187041	298852	29.75%	3.917%
6	2.386	209	213	219	rVV2	7550	12471	1.24%	0.163%
7	2.434	219	221	222	rVB	1147	587	0.06%	0.008%
8	2.453	222	224	226	rVB3	794	600	0.06%	0.008%
9	2.709	262	266	267	rBV3	622	829	0.08%	0.011%
10	2.782	276	278	283	rVB6	1730	2386	0.24%	0.031%
11	2.940	297	304	315	rVB3	6271	16265	1.62%	0.213%
12	3.434	378	385	391	rBV7	3243	7507	0.75%	0.098%
13	3.544	400	403	405	rVB4	575	463	0.05%	0.006%
14	3.562	405	406	409	rBV2	487	578	0.06%	0.008%
15	3.629	415	417	421	rVB2	593	892	0.09%	0.012%
16	3.703	427	429	433	rVB3	456	589	0.06%	0.008%
17	3.733	433	434	439	rBV4	596	627	0.06%	0.008%
18	3.818	447	448	452	rVB4	637	753	0.07%	0.010%
19	4.093	490	493	496	rVV4	458	623	0.06%	0.008%
20	4.117	496	497	501	rVB2	640	541	0.05%	0.007%
21	4.288	523	525	529	rBV3	429	559	0.06%	0.007%
22	4.373	536	539	541	rBV2	688	859	0.09%	0.011%
23	4.458	545	553	573	rBV2	69312	218987	21.80%	2.870%
24	4.739	597	599	601	rBV2	634	504	0.05%	0.007%
25	5.056	639	651	666	rVV2	137025	426300	42.43%	5.587%
26	5.391	702	706	707	rVB2	850	1045	0.10%	0.014%
27	5.410	707	709	711	rBV	583	542	0.05%	0.007%
28	5.483	718	721	724	rVB3	480	532	0.05%	0.007%
29	5.672	749	752	753	rBV2	665	631	0.06%	0.008%
30	5.763	764	767	770	rVB2	549	725	0.07%	0.010%
31	5.964	788	800	819	rBV3	337603	1004630	100.00%	13.167%
32	6.135	826	828	831	rVB3	886	559	0.06%	0.007%
33	6.269	848	850	852	rBV3	656	514	0.05%	0.007%
34	6.348	858	863	873	rVB4	5519	13443	1.34%	0.176%
35	6.476	882	884	888	rVB4	1023	1046	0.10%	0.014%
36	6.513	888	890	891	rBV	621	560	0.06%	0.007%

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Integrator: RTE

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Title : VOC Analysis

37	6.635	909	910	913	rBV2	463	534	0.05%	0.007%
38	6.757	922	930	950	rBV	246076	607095	60.43%	7.957%
39	6.995	968	969	972	rBV2	802	483	0.05%	0.006%
40	7.117	984	989	990	rBV4	1841	3002	0.30%	0.039%
41	7.306	1009	1020	1034	rBV	208580	469349	46.72%	6.152%
42	7.464	1045	1046	1047	rBV	944	558	0.06%	0.007%
43	7.574	1062	1064	1066	rBV2	628	582	0.06%	0.008%
44	7.653	1071	1077	1081	rBV3	2610	5344	0.53%	0.070%
45	7.799	1096	1101	1115	rBV	57472	108162	10.77%	1.418%
46	7.940	1122	1124	1126	rBV2	823	638	0.06%	0.008%
47	8.165	1159	1161	1163	rBV2	576	530	0.05%	0.007%
48	8.324	1181	1187	1199	rBV	125547	209818	20.89%	2.750%
49	8.549	1219	1224	1234	rBV	15878	30099	3.00%	0.394%
50	8.647	1234	1240	1254	rVV	464911	731986	72.86%	9.594%
51	8.952	1285	1290	1303	rBV2	92424	155068	15.44%	2.032%
52	9.244	1334	1338	1347	rBV	23535	35255	3.51%	0.462%
53	9.384	1356	1361	1374	rBV	310300	471500	46.93%	6.180%
54	9.488	1374	1378	1390	rVV	26838	42712	4.25%	0.560%
55	9.586	1390	1394	1407	rVB	10357	19651	1.96%	0.258%
56	9.787	1424	1427	1429	rBV2	699	778	0.08%	0.010%
57	9.817	1429	1432	1437	rVV5	779	1419	0.14%	0.019%
58	9.915	1443	1448	1458	rBV	58241	80923	8.06%	1.061%
59	10.055	1465	1471	1487	rBV	487650	700311	69.71%	9.179%
60	10.494	1539	1543	1545	rBV3	695	550	0.05%	0.007%
61	10.524	1545	1548	1549	rBV2	801	776	0.08%	0.010%
62	10.652	1565	1569	1573	rBV6	1986	3129	0.31%	0.041%
63	10.750	1584	1585	1589	rBV3	706	673	0.07%	0.009%
64	10.896	1608	1609	1611	rBV2	683	570	0.06%	0.007%
65	11.055	1633	1635	1639	rBV3	397	599	0.06%	0.008%
66	11.116	1644	1645	1651	rVB2	642	556	0.06%	0.007%
67	11.189	1652	1657	1667	rBV	370220	477041	47.48%	6.252%
68	11.506	1707	1709	1711	rVV3	506	553	0.06%	0.007%
69	11.634	1726	1730	1733	rBV3	471	906	0.09%	0.012%
70	11.713	1741	1743	1747	rVB3	644	647	0.06%	0.008%
71	11.945	1777	1781	1783	rBV4	552	839	0.08%	0.011%
72	12.018	1788	1793	1804	rBV	421896	556848	55.43%	7.298%
73	12.317	1837	1842	1852	rBV	469886	596209	59.35%	7.814%
74	12.591	1884	1887	1890	rBV3	641	952	0.09%	0.012%
75	12.762	1911	1915	1920	rVB4	967	1885	0.19%	0.025%
76	12.798	1920	1921	1924	rBV2	547	508	0.05%	0.007%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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

77	12.908	1937	1939	1943	rBV3	781	753	0.07%	0.010%
78	13.311	2001	2005	2007	rVV3	527	784	0.08%	0.010%
79	13.372	2013	2015	2018	rBV2	416	496	0.05%	0.007%
80	13.573	2045	2048	2050	rVB2	821	791	0.08%	0.010%
81	13.603	2050	2053	2055	rBV2	685	846	0.08%	0.011%
82	13.737	2073	2075	2079	rBV3	580	585	0.06%	0.008%
83	13.835	2090	2091	2094	rVB2	925	744	0.07%	0.010%
84	13.859	2094	2095	2096	rBV	708	450	0.04%	0.006%
85	13.926	2104	2106	2107	rVB2	672	442	0.04%	0.006%
86	14.115	2135	2137	2138	rBV2	620	611	0.06%	0.008%
87	14.195	2147	2150	2151	rBV3	700	608	0.06%	0.008%
88	14.213	2151	2153	2155	rVB2	913	749	0.07%	0.010%
89	14.231	2155	2156	2158	rBV	748	607	0.06%	0.008%
90	14.310	2166	2169	2170	rBV2	549	600	0.06%	0.008%
91	14.451	2189	2192	2193	rBV3	750	829	0.08%	0.011%
92	14.682	2228	2230	2236	rVB2	764	1019	0.10%	0.013%
93	14.774	2242	2245	2247	rBV3	526	685	0.07%	0.009%
94	15.042	2287	2289	2291	rVB2	698	539	0.05%	0.007%
95	15.139	2300	2305	2307	rBV4	700	1336	0.13%	0.018%
96	15.316	2332	2334	2335	rVB	925	499	0.05%	0.007%
97	15.402	2346	2348	2349	rVB	975	490	0.05%	0.006%
98	16.286	2492	2493	2494	rBV	830	501	0.05%	0.007%
99	16.536	2533	2534	2536	rBV2	705	457	0.05%	0.006%
100	16.767	2569	2572	2574	rBV3	722	770	0.08%	0.010%

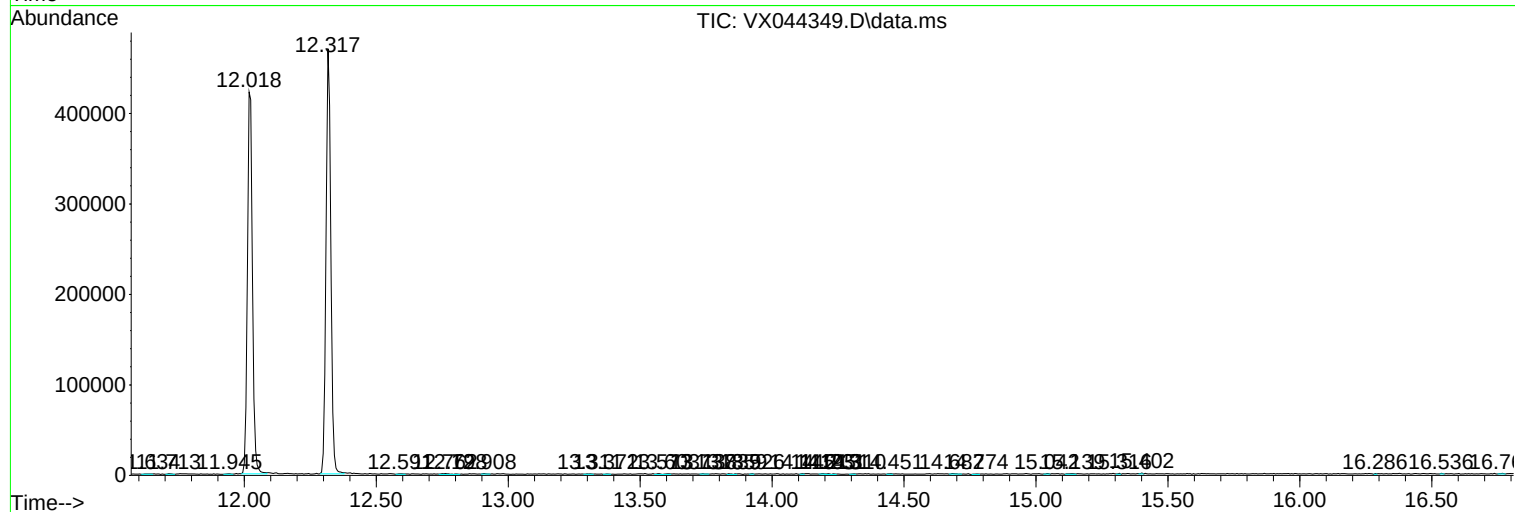
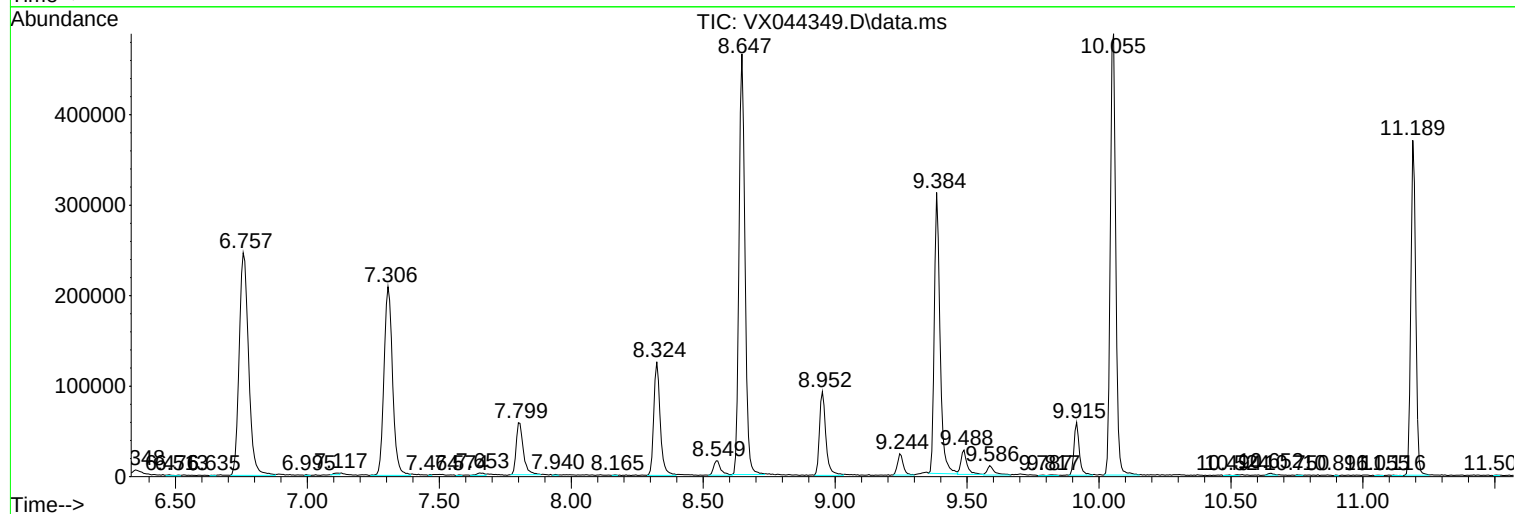
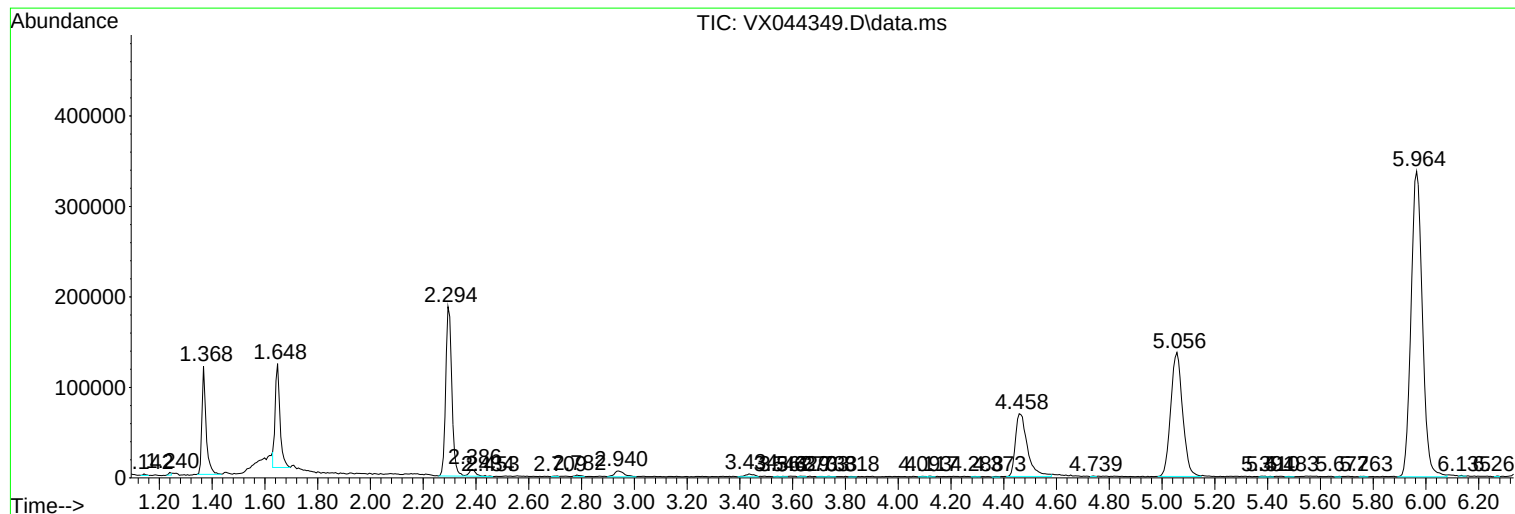
Sum of corrected areas: 7629723

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Instrument :
MSVOA_X
ClientSampleId :
C0AW0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.M
Quant Title : VOC Analysis

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



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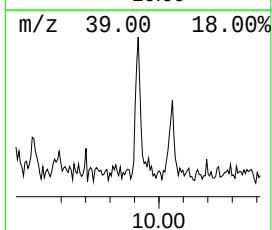
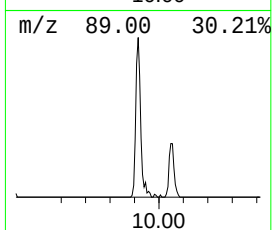
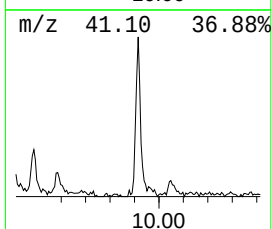
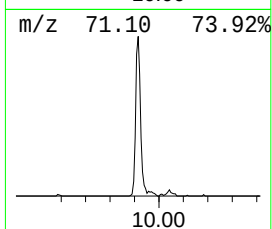
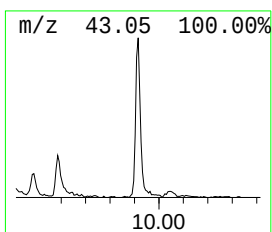
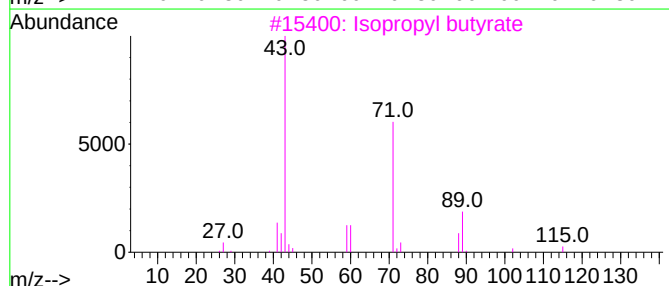
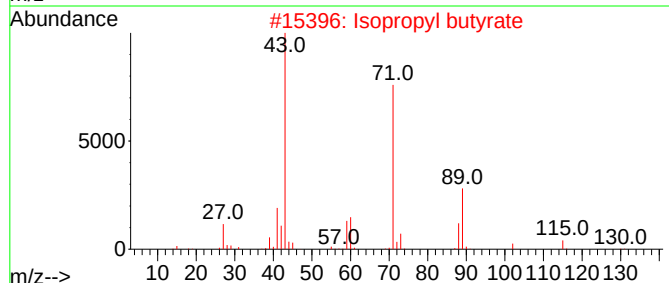
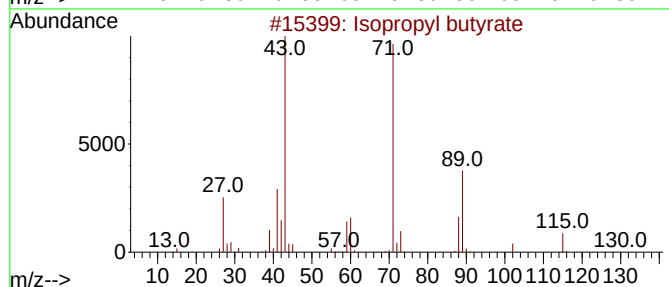
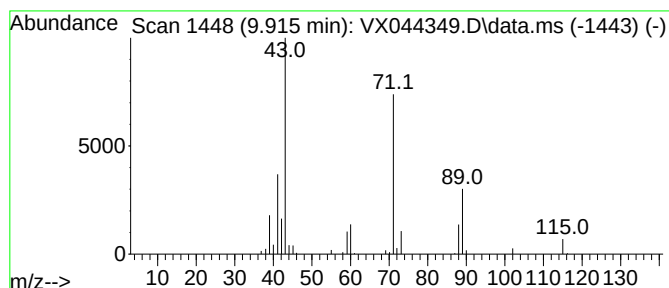
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

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	5.78 ug/L	80923	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			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	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	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl butyrate	9.915	5.8	ug/L	80923	2	10.055	700311	50.0