

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
 Data File : VX044517.D
 Acq On : 27 Dec 2024 13:49
 Operator : JC/MD
 Sample : PB165836TB 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VLEB836

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\SFAMXML120524WMA.M
 Title : VOC Analysis

Signal : TIC: VX044517.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	22	25	27	rBV	3776	4779	0.50%	0.067%
2	1.368	43	46	57	rBV	111492	137730	14.29%	1.924%
3	1.642	88	91	104	rVB	94454	155269	16.11%	2.169%
4	2.294	192	198	209	rBV	203096	314525	32.63%	4.393%
5	2.483	226	229	230	rBV2	520	559	0.06%	0.008%
6	2.776	272	277	284	rVB6	1760	3372	0.35%	0.047%
7	2.941	299	304	315	rVV2	6342	15282	1.59%	0.213%
8	3.123	332	334	337	rVV4	600	753	0.08%	0.011%
9	3.154	337	339	341	rVV2	532	448	0.05%	0.006%
10	3.239	350	353	357	rVB3	579	736	0.08%	0.010%
11	3.306	360	364	365	rBV2	485	472	0.05%	0.007%
12	3.379	372	376	378	rBV2	431	562	0.06%	0.008%
13	3.440	379	386	392	rVB7	2557	6412	0.67%	0.090%
14	3.581	404	409	414	rBV6	1107	2639	0.27%	0.037%
15	3.782	439	442	444	rBV2	446	564	0.06%	0.008%
16	3.928	462	466	469	rBV3	404	547	0.06%	0.008%
17	4.270	519	522	523	rBV2	547	500	0.05%	0.007%
18	4.330	529	532	533	rBV	429	421	0.04%	0.006%
19	4.459	546	553	571	rBV	51040	162336	16.84%	2.267%
20	5.050	638	650	674	rVV2	144470	517016	53.63%	7.221%
21	5.294	688	690	694	rVB	520	443	0.05%	0.006%
22	5.379	700	704	706	rBV3	625	1066	0.11%	0.015%
23	5.483	718	721	723	rVB2	405	464	0.05%	0.006%
24	5.525	723	728	729	rBV4	694	1239	0.13%	0.017%
25	5.568	733	735	737	rVB2	765	481	0.05%	0.007%
26	5.849	779	781	785	rBV4	404	439	0.05%	0.006%
27	5.958	788	799	817	rBV2	329805	964008	100.00%	13.464%
28	6.348	857	863	875	rVV4	5495	15319	1.59%	0.214%
29	6.757	921	930	943	rBV	195363	465307	48.27%	6.499%
30	7.013	970	972	975	rBV2	463	600	0.06%	0.008%
31	7.123	979	990	999	rBV9	5970	16788	1.74%	0.234%
32	7.190	999	1001	1002	rBV	696	460	0.05%	0.006%
33	7.306	1011	1020	1033	rBV	198759	439040	45.54%	6.132%
34	7.476	1046	1048	1050	rBV2	507	541	0.06%	0.008%
35	7.543	1057	1059	1062	rVB3	673	591	0.06%	0.008%
36	7.592	1062	1067	1069	rBV3	545	1031	0.11%	0.014%

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 Title : VOC Analysis

37	7.671	1074	1080	1084	rBV3	1595	3333	0.35%	0.047%
38	7.799	1096	1101	1113	rBV	66857	128140	13.29%	1.790%
39	8.263	1173	1177	1180	rBV4	612	1172	0.12%	0.016%
40	8.324	1181	1187	1197	rBV	116992	193845	20.11%	2.707%
41	8.549	1219	1224	1233	rBV	15301	27791	2.88%	0.388%
42	8.647	1233	1240	1253	rBV	458280	731214	75.85%	10.213%
43	8.952	1284	1290	1300	rBV2	91191	156461	16.23%	2.185%
44	9.244	1333	1338	1348	rVV	23821	36431	3.78%	0.509%
45	9.342	1348	1354	1356	rVV5	4563	7352	0.76%	0.103%
46	9.384	1356	1361	1374	rVV	240339	377171	39.13%	5.268%
47	9.488	1374	1378	1389	rVV	34658	56147	5.82%	0.784%
48	9.586	1389	1394	1404	rVB	21986	35395	3.67%	0.494%
49	9.750	1419	1421	1422	rBV2	546	485	0.05%	0.007%
50	9.762	1422	1423	1424	rBV	672	452	0.05%	0.006%
51	9.915	1441	1448	1458	rBV	68357	96736	10.03%	1.351%
52	10.049	1465	1470	1482	rBV	371934	542879	56.31%	7.582%
53	10.208	1495	1496	1500	rVB3	790	570	0.06%	0.008%
54	10.390	1524	1526	1529	rBV4	364	437	0.05%	0.006%
55	10.567	1552	1555	1557	rBV3	794	942	0.10%	0.013%
56	10.646	1563	1568	1573	rBV3	3680	6276	0.65%	0.088%
57	10.835	1597	1599	1603	rVB2	418	492	0.05%	0.007%
58	10.976	1617	1622	1624	rVV2	782	1111	0.12%	0.016%
59	11.189	1652	1657	1668	rBV	327473	430684	44.68%	6.015%
60	11.299	1674	1675	1676	rBV	616	433	0.04%	0.006%
61	11.372	1684	1687	1691	rBV4	685	1256	0.13%	0.018%
62	11.543	1711	1715	1718	rVB3	376	645	0.07%	0.009%
63	11.567	1718	1719	1722	rBV	508	575	0.06%	0.008%
64	11.634	1728	1730	1735	rBV4	714	1059	0.11%	0.015%
65	11.762	1749	1751	1754	rVB2	772	874	0.09%	0.012%
66	11.786	1754	1755	1758	rBV2	603	680	0.07%	0.009%
67	11.951	1779	1782	1784	rBV2	678	772	0.08%	0.011%
68	11.982	1784	1787	1788	rBV2	870	812	0.08%	0.011%
69	12.018	1788	1793	1808	rBV	363220	460235	47.74%	6.428%
70	12.317	1837	1842	1849	rVV	473777	590889	61.30%	8.253%
71	12.628	1892	1893	1896	rBV3	506	548	0.06%	0.008%
72	12.707	1904	1906	1907	rVV	614	438	0.05%	0.006%
73	12.768	1911	1916	1920	rBV6	2098	3779	0.39%	0.053%
74	12.829	1923	1926	1927	rBV	677	508	0.05%	0.007%
75	13.189	1984	1985	1987	rBV	514	415	0.04%	0.006%
76	13.646	2057	2060	2063	rBV3	703	930	0.10%	0.013%

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

77	13.707	2066	2070	2072	rBV4	544	677	0.07%	0.009%
78	13.975	2112	2114	2116	rBV2	856	802	0.08%	0.011%
79	14.134	2136	2140	2144	rVB2	3628	4810	0.50%	0.067%
80	14.499	2196	2200	2202	rVB2	954	1005	0.10%	0.014%
81	14.560	2208	2210	2212	rBV3	576	456	0.05%	0.006%
82	14.579	2212	2213	2216	rVB2	833	628	0.07%	0.009%
83	14.609	2216	2218	2220	rBV2	929	987	0.10%	0.014%
84	14.786	2245	2247	2250	rVB3	939	778	0.08%	0.011%
85	14.981	2278	2279	2282	rVB2	780	442	0.05%	0.006%
86	15.109	2298	2300	2301	rBV2	571	418	0.04%	0.006%
87	15.201	2312	2315	2316	rBV3	684	737	0.08%	0.010%
88	15.316	2332	2334	2335	rBV2	710	622	0.06%	0.009%
89	15.487	2358	2362	2367	rVB6	2058	3533	0.37%	0.049%
90	15.530	2367	2369	2371	rBV2	1109	1181	0.12%	0.016%
91	15.591	2376	2379	2380	rBV2	678	811	0.08%	0.011%
92	15.658	2388	2390	2394	rVB3	741	778	0.08%	0.011%
93	15.700	2394	2397	2399	rBV4	627	805	0.08%	0.011%
94	16.249	2486	2487	2489	rBV	843	815	0.08%	0.011%
95	16.371	2505	2507	2511	rVV4	1988	2469	0.26%	0.034%
96	16.426	2514	2516	2518	rVB2	702	618	0.06%	0.009%
97	16.530	2531	2533	2534	rBV2	741	419	0.04%	0.006%
98	16.615	2542	2547	2550	rVB4	790	1400	0.15%	0.020%
99	16.651	2550	2553	2556	rBV3	1047	1145	0.12%	0.016%
100	16.725	2563	2565	2567	rVB2	706	532	0.06%	0.007%

Sum of corrected areas: 7159971

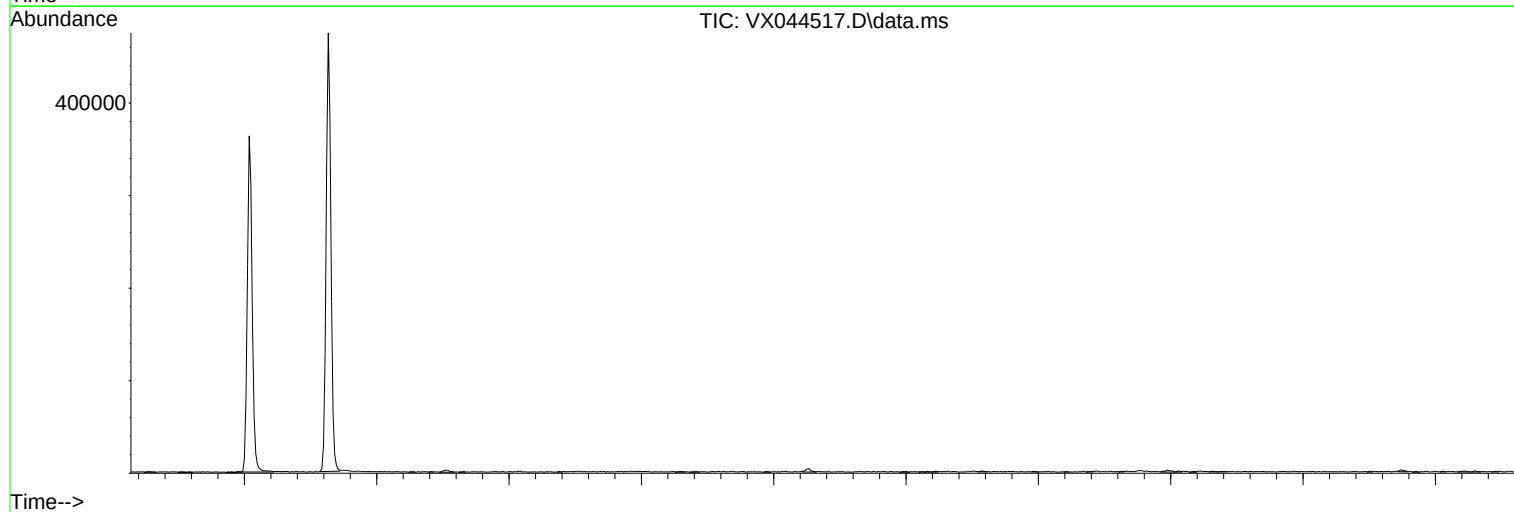
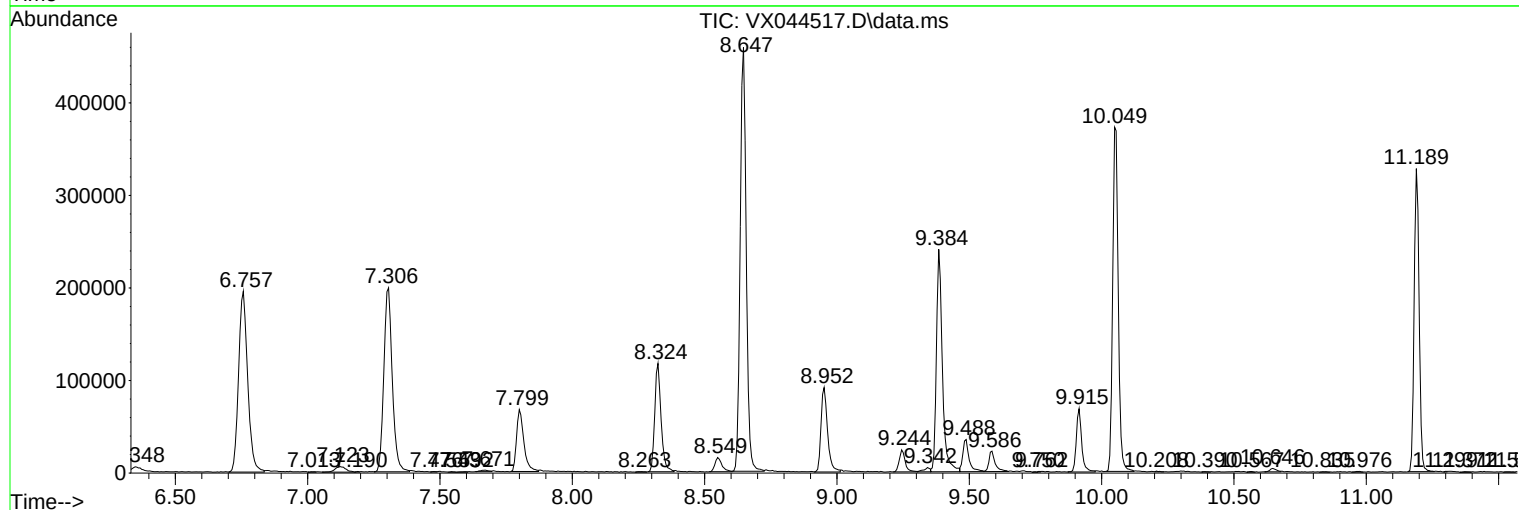
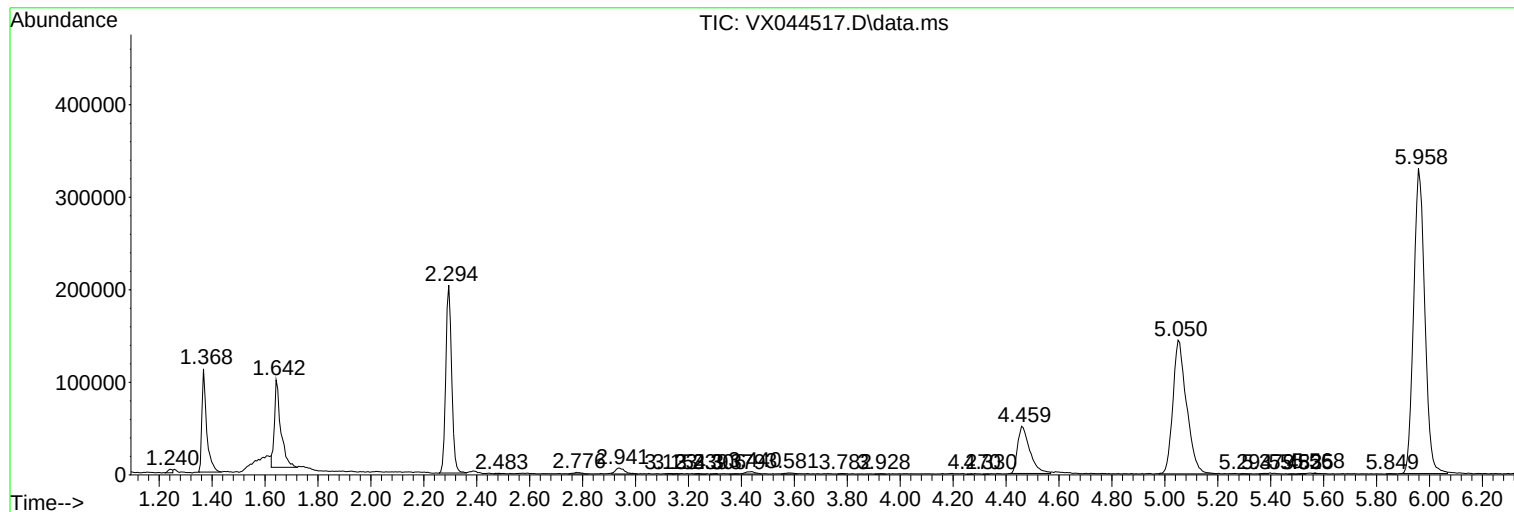
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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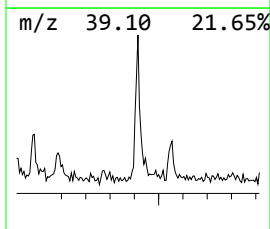
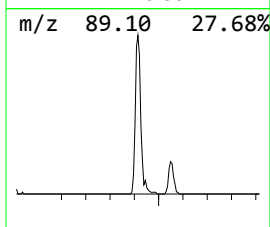
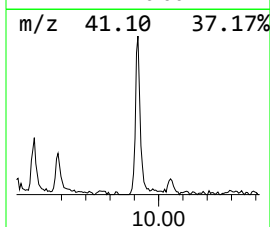
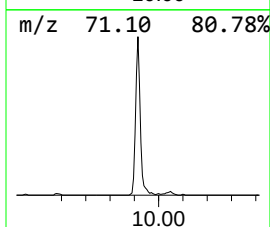
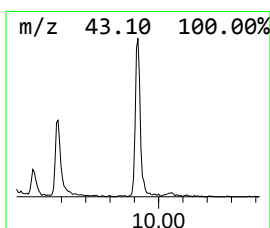
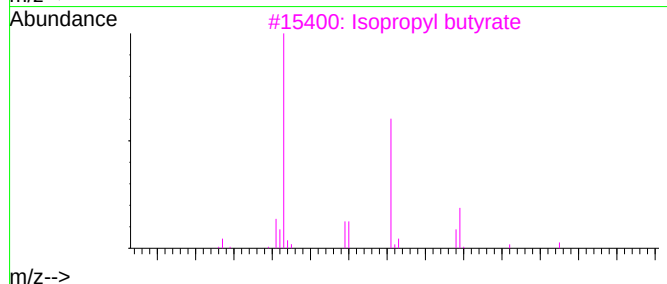
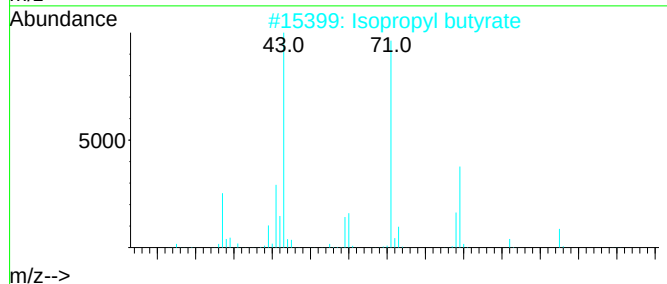
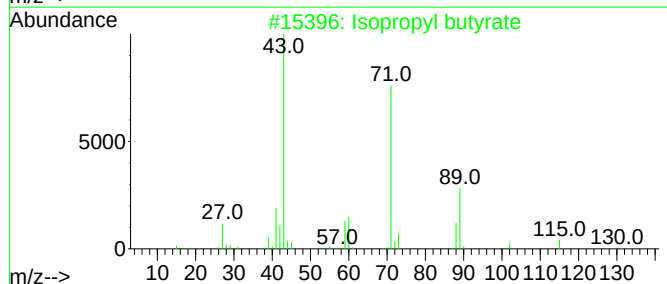
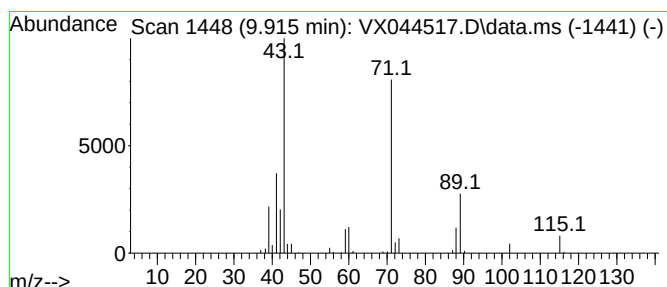
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	8.91 ug/L	96736	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	86
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	80
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
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	8.9	ug/L	96736	2	10.055	542879	50.0