

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
 Data File : VX044518.D
 Acq On : 27 Dec 2024 14:12
 Operator : JC/MD
 Sample : P5326-04 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YE682

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: VX044518.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	32	rBV2	4616	7342	0.71%	0.099%
2	1.368	42	46	55	rBV	135492	153458	14.86%	2.059%
3	1.593	69	83	84	rBV3	16612	54165	5.25%	0.727%
4	1.648	88	92	100	rVB	109767	152815	14.80%	2.050%
5	2.294	192	198	209	rBV	214119	343191	33.24%	4.605%
6	2.380	209	212	218	rVB2	3139	5126	0.50%	0.069%
7	2.489	229	230	231	rBV	694	401	0.04%	0.005%
8	2.563	235	242	247	rVB5	1082	2638	0.26%	0.035%
9	2.599	247	248	253	rVB2	608	619	0.06%	0.008%
10	2.654	255	257	259	rBV3	445	410	0.04%	0.006%
11	2.678	259	261	264	rBV	551	595	0.06%	0.008%
12	2.782	274	278	280	rBV3	1495	1871	0.18%	0.025%
13	2.941	296	304	316	rBV	8630	21739	2.11%	0.292%
14	3.044	318	321	324	rBV3	697	874	0.08%	0.012%
15	3.099	328	330	331	rBV	598	392	0.04%	0.005%
16	3.440	379	386	392	rVB6	3454	8171	0.79%	0.110%
17	3.575	405	408	409	rVV2	497	427	0.04%	0.006%
18	3.800	443	445	449	rBV3	453	582	0.06%	0.008%
19	3.922	463	465	469	rBV3	560	809	0.08%	0.011%
20	4.081	489	491	492	rBV2	622	461	0.04%	0.006%
21	4.160	502	504	505	rBV2	540	451	0.04%	0.006%
22	4.233	513	516	517	rBV3	508	436	0.04%	0.006%
23	4.452	544	552	570	rBV	61386	191735	18.57%	2.573%
24	4.897	622	625	627	rVB3	671	526	0.05%	0.007%
25	5.044	638	649	668	rBV2	135816	435517	42.18%	5.844%
26	5.233	677	680	683	rBV3	592	685	0.07%	0.009%
27	5.263	683	685	689	rVB4	459	469	0.05%	0.006%
28	5.397	702	707	711	rBV5	922	1968	0.19%	0.026%
29	5.519	724	727	728	rBV3	617	681	0.07%	0.009%
30	5.544	728	731	734	rVV3	699	1157	0.11%	0.016%
31	5.721	756	760	763	rBV3	480	846	0.08%	0.011%
32	5.958	789	799	822	rBV3	337532	1032478	100.00%	13.854%
33	6.208	838	840	841	rVB2	601	429	0.04%	0.006%
34	6.348	857	863	873	rBV4	5218	13242	1.28%	0.178%
35	6.659	912	914	917	rBV3	609	825	0.08%	0.011%
36	6.757	921	930	945	rBV	197385	475752	46.08%	6.384%

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 Title : VOC Analysis

37	6.989	967	968	971	rVB	678	489	0.05%	0.007%
38	7.123	983	990	1000	rVB8	8602	22533	2.18%	0.302%
39	7.239	1005	1009	1010	rBV2	517	502	0.05%	0.007%
40	7.306	1011	1020	1037	rBV	203906	463339	44.88%	6.217%
41	7.659	1074	1078	1083	rBV4	2087	3436	0.33%	0.046%
42	7.799	1096	1101	1116	rBV	67042	129392	12.53%	1.736%
43	8.074	1145	1146	1149	rBV3	510	396	0.04%	0.005%
44	8.202	1163	1167	1168	rBV2	280	452	0.04%	0.006%
45	8.324	1181	1187	1204	rBV	122448	212946	20.62%	2.857%
46	8.470	1210	1211	1214	rVB2	566	526	0.05%	0.007%
47	8.507	1214	1217	1218	rBV2	674	724	0.07%	0.010%
48	8.549	1219	1224	1233	rVV	15624	27360	2.65%	0.367%
49	8.647	1234	1240	1251	rBV	498205	786682	76.19%	10.556%
50	8.952	1284	1290	1299	rBV2	97475	160582	15.55%	2.155%
51	9.159	1322	1324	1327	rVB2	366	375	0.04%	0.005%
52	9.214	1330	1333	1334	rBV2	963	1035	0.10%	0.014%
53	9.244	1334	1338	1348	rVV	21773	34544	3.35%	0.464%
54	9.384	1356	1361	1372	rBV	261770	402939	39.03%	5.407%
55	9.482	1374	1377	1389	rVB	33183	49200	4.77%	0.660%
56	9.580	1390	1393	1407	rVV	16526	28609	2.77%	0.384%
57	9.701	1410	1413	1416	rVB3	1408	1881	0.18%	0.025%
58	9.872	1439	1441	1442	rBV	657	490	0.05%	0.007%
59	9.915	1442	1448	1455	rVV	58238	84222	8.16%	1.130%
60	10.049	1465	1470	1483	rBV	393274	560791	54.32%	7.525%
61	10.293	1507	1510	1512	rBV2	1216	1307	0.13%	0.018%
62	10.409	1527	1529	1533	rBV3	730	952	0.09%	0.013%
63	10.518	1543	1547	1548	rBV3	675	935	0.09%	0.013%
64	10.610	1561	1562	1564	rBV2	446	394	0.04%	0.005%
65	10.646	1564	1568	1578	rVB7	3303	6710	0.65%	0.090%
66	10.970	1617	1621	1622	rBV3	543	625	0.06%	0.008%
67	11.061	1634	1636	1637	rVB	757	387	0.04%	0.005%
68	11.140	1645	1649	1651	rBV3	695	1105	0.11%	0.015%
69	11.189	1652	1657	1667	rVV	370634	465634	45.10%	6.248%
70	11.427	1694	1696	1699	rVV2	573	606	0.06%	0.008%
71	11.451	1699	1700	1704	rVB3	737	744	0.07%	0.010%
72	11.500	1706	1708	1711	rVB3	573	551	0.05%	0.007%
73	11.640	1728	1731	1732	rVB2	492	392	0.04%	0.005%
74	11.762	1749	1751	1752	rBV	754	512	0.05%	0.007%
75	11.975	1784	1786	1788	rBV3	607	522	0.05%	0.007%
76	12.018	1788	1793	1804	rBV	362613	454431	44.01%	6.098%

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77	12.317	1837	1842	1854	rBV	480218	605324	58.63%	8.122%
78	12.549	1878	1880	1882	rVV2	449	471	0.05%	0.006%
79	12.756	1911	1914	1920	rVB2	2448	3484	0.34%	0.047%
80	12.866	1929	1932	1934	rBV2	505	728	0.07%	0.010%
81	13.079	1964	1967	1970	rBV4	550	696	0.07%	0.009%
82	13.122	1972	1974	1976	rBV2	476	497	0.05%	0.007%
83	13.201	1986	1987	1989	rVB2	651	399	0.04%	0.005%
84	13.561	2044	2046	2050	rBV4	565	725	0.07%	0.010%
85	13.786	2081	2083	2085	rBV3	422	389	0.04%	0.005%
86	13.865	2094	2096	2099	rBV2	567	566	0.05%	0.008%
87	13.908	2102	2103	2107	rVB2	603	456	0.04%	0.006%
88	13.945	2107	2109	2111	rBV3	399	400	0.04%	0.005%
89	14.128	2133	2139	2144	rBV	3778	6241	0.60%	0.084%
90	14.219	2152	2154	2155	rBV	617	513	0.05%	0.007%
91	14.292	2163	2166	2167	rBV2	690	525	0.05%	0.007%
92	14.426	2186	2188	2190	rBV3	493	514	0.05%	0.007%
93	14.487	2197	2198	2201	rBV3	342	384	0.04%	0.005%
94	14.981	2277	2279	2280	rBV2	842	749	0.07%	0.010%
95	15.390	2342	2346	2353	rVB5	1864	3759	0.36%	0.050%
96	15.505	2364	2365	2367	rBV2	1017	895	0.09%	0.012%
97	15.981	2442	2443	2444	rBV	719	474	0.05%	0.006%
98	16.243	2485	2486	2489	rBV3	681	654	0.06%	0.009%
99	16.371	2504	2507	2509	rBV2	749	908	0.09%	0.012%
100	16.414	2513	2514	2515	rBV	623	392	0.04%	0.005%

Sum of corrected areas: 7452678

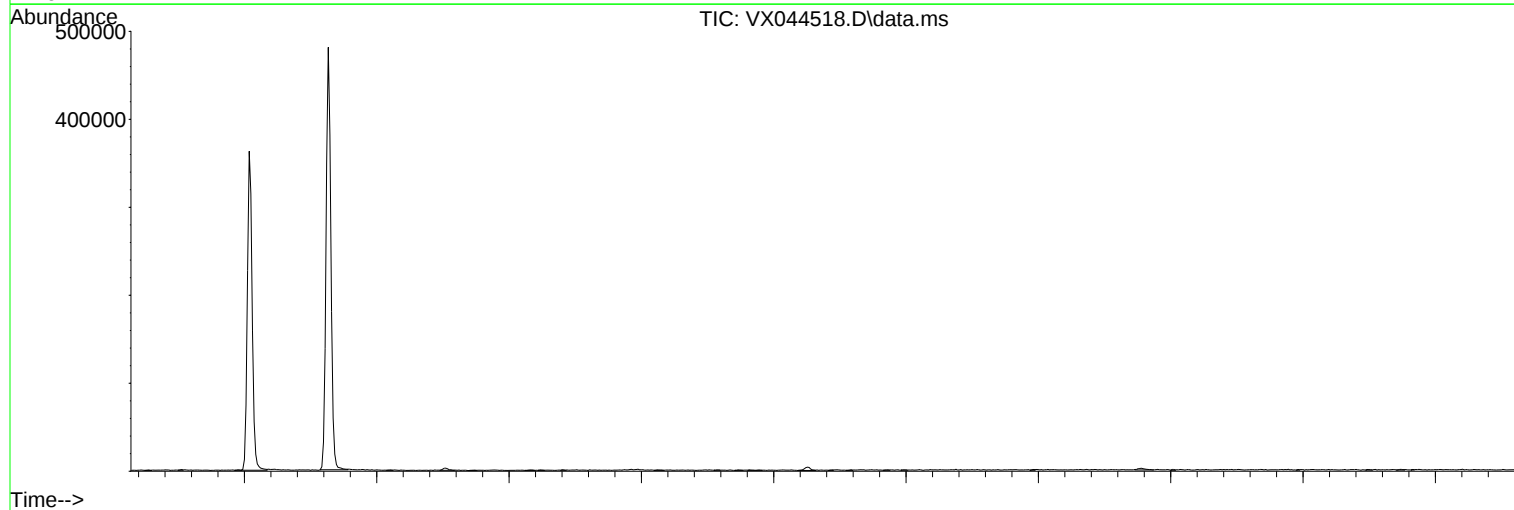
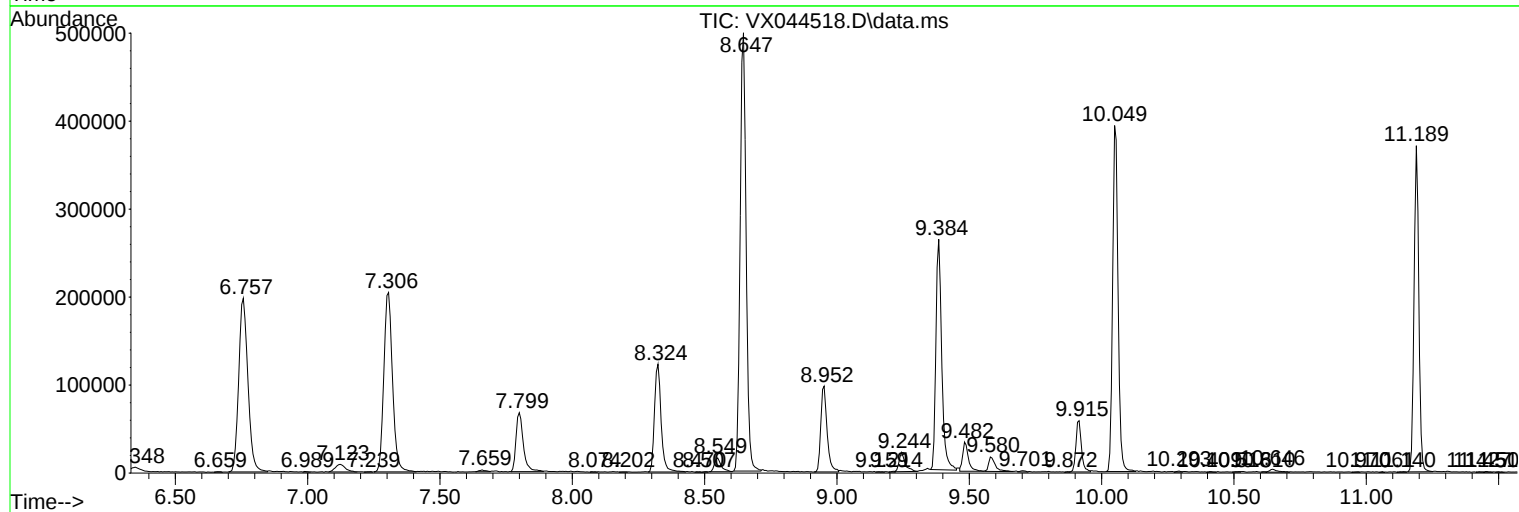
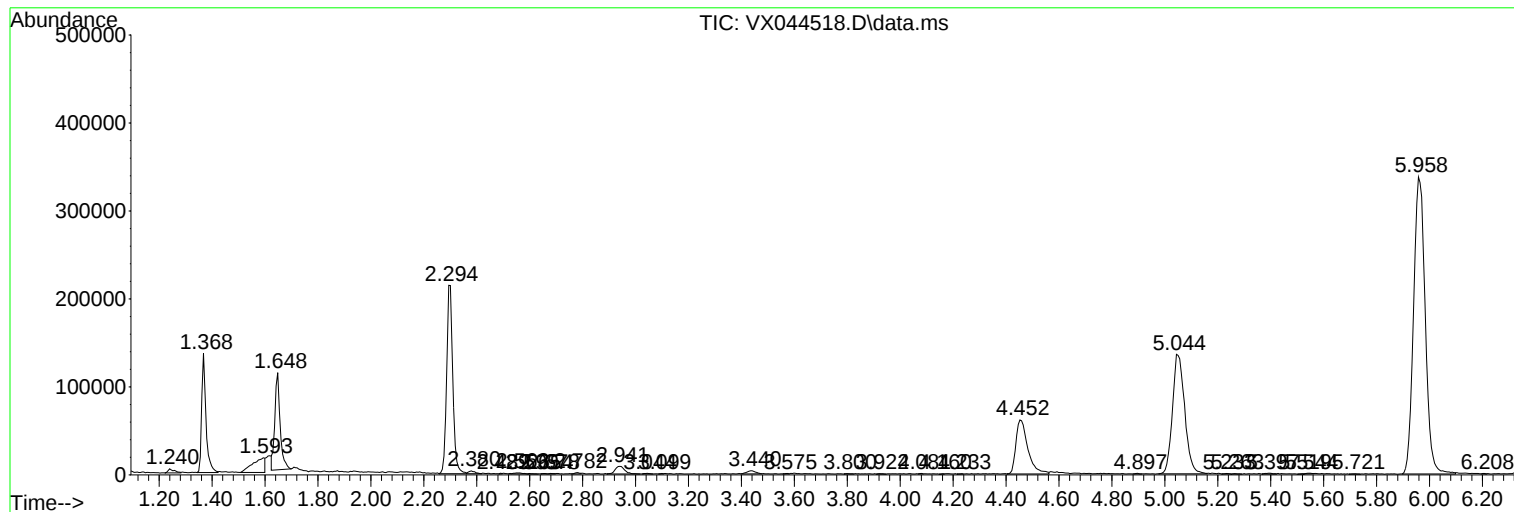
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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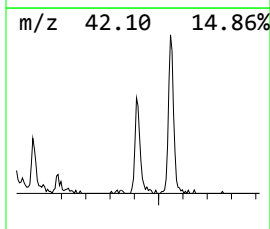
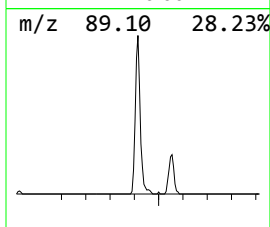
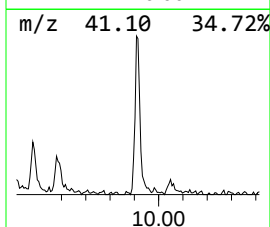
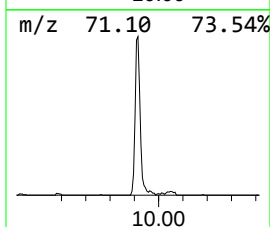
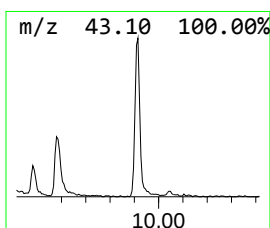
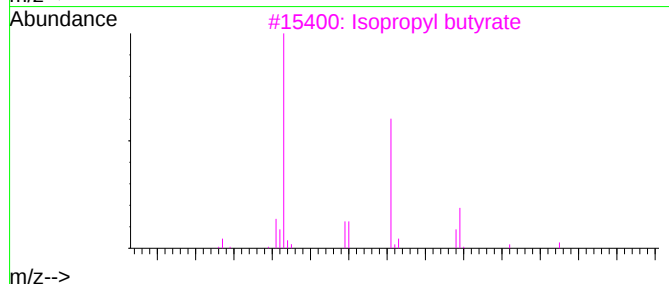
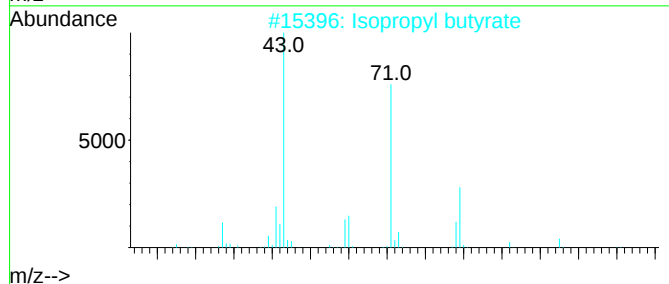
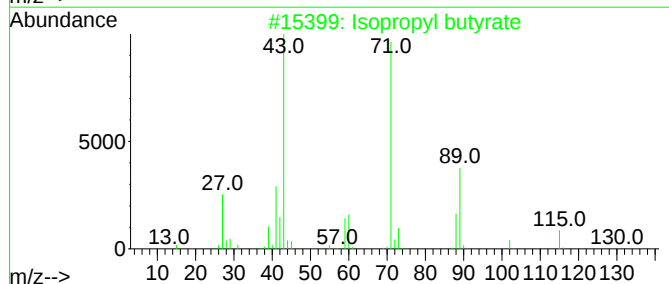
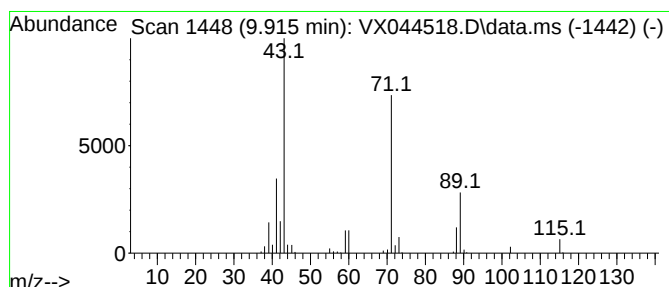
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	7.51 ug/L	84222	Chlorobenzene-d5	10.049

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	78
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl butyrate	9.915	7.5	ug/L	84222	2	10.049	560791	50.0