

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
 Data File : VX044520.D
 Acq On : 27 Dec 2024 14:58
 Operator : JC/MD
 Sample : P5326-07 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YE686

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: VX044520.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	31	rBV3	4592	8162	0.84%	0.110%
2	1.368	42	46	56	rBV	134915	148043	15.19%	1.992%
3	1.642	88	91	104	rVB	110175	153367	15.74%	2.063%
4	2.294	192	198	208	rBV	203413	321710	33.02%	4.328%
5	2.569	241	243	247	rVB4	1007	1223	0.13%	0.016%
6	2.617	247	251	252	rBV3	709	710	0.07%	0.010%
7	2.788	274	279	284	rVB6	1852	3502	0.36%	0.047%
8	2.934	299	303	311	rVB2	3619	8245	0.85%	0.111%
9	3.123	333	334	339	rVB2	580	736	0.08%	0.010%
10	3.190	342	345	346	rBV2	529	548	0.06%	0.007%
11	3.294	360	362	364	rBV2	693	611	0.06%	0.008%
12	3.434	381	385	391	rVB4	2517	4700	0.48%	0.063%
13	3.526	396	400	402	rBV3	410	636	0.07%	0.009%
14	3.575	403	408	414	rBV2	4394	10102	1.04%	0.136%
15	3.733	432	434	437	rBV2	501	592	0.06%	0.008%
16	3.837	449	451	455	rVB4	706	832	0.09%	0.011%
17	3.873	455	457	459	rBV2	553	510	0.05%	0.007%
18	3.934	466	467	469	rBV2	619	445	0.05%	0.006%
19	4.062	486	488	489	rVB	731	486	0.05%	0.007%
20	4.081	489	491	494	rBV2	740	828	0.08%	0.011%
21	4.178	506	507	510	rBV3	496	456	0.05%	0.006%
22	4.288	523	525	527	rBV2	581	451	0.05%	0.006%
23	4.459	544	553	567	rBV	57969	179071	18.38%	2.409%
24	4.672	586	588	589	rBV	671	536	0.06%	0.007%
25	4.898	622	625	626	rBV	996	897	0.09%	0.012%
26	5.044	638	649	669	rVV	131997	417463	42.84%	5.616%
27	5.269	684	686	687	rBV2	465	432	0.04%	0.006%
28	5.562	733	734	739	rVB2	1074	794	0.08%	0.011%
29	5.739	761	763	765	rVB2	502	463	0.05%	0.006%
30	5.794	769	772	774	rVB3	531	536	0.06%	0.007%
31	5.964	789	800	815	rBV3	329173	974431	100.00%	13.109%
32	6.348	857	863	871	rBV3	5672	15570	1.60%	0.209%
33	6.757	922	930	942	rBV	190273	470427	48.28%	6.329%
34	6.982	965	967	971	rBV3	649	943	0.10%	0.013%
35	7.123	983	990	998	rBV8	4891	12696	1.30%	0.171%
36	7.214	1002	1005	1007	rBV2	717	796	0.08%	0.011%

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

37	7.306	1011	1020	1036	rBV	195073	442312	45.39%	5.950%
38	7.476	1046	1048	1052	rBV5	864	1106	0.11%	0.015%
39	7.531	1054	1057	1058	rBV3	691	684	0.07%	0.009%
40	7.580	1061	1065	1066	rBV3	593	706	0.07%	0.009%
41	7.629	1071	1073	1074	rBV2	640	513	0.05%	0.007%
42	7.659	1074	1078	1083	rBV	2079	4499	0.46%	0.061%
43	7.799	1095	1101	1116	rBV	87955	159936	16.41%	2.152%
44	8.324	1180	1187	1197	rBV	121771	205143	21.05%	2.760%
45	8.549	1217	1224	1233	rBV	20185	36121	3.71%	0.486%
46	8.647	1234	1240	1255	rVB	472476	751242	77.10%	10.106%
47	8.952	1284	1290	1300	rBV2	99871	165228	16.96%	2.223%
48	9.244	1333	1338	1347	rBV	28907	42584	4.37%	0.573%
49	9.342	1351	1354	1356	rVV4	4100	5075	0.52%	0.068%
50	9.385	1356	1361	1373	rVV	275566	401441	41.20%	5.400%
51	9.482	1373	1377	1384	rVB	41181	58580	6.01%	0.788%
52	9.580	1389	1393	1401	rVB	23391	36044	3.70%	0.485%
53	9.775	1423	1425	1426	rBV	467	477	0.05%	0.006%
54	9.854	1436	1438	1439	rBV	799	469	0.05%	0.006%
55	9.915	1443	1448	1456	rBV	84313	114589	11.76%	1.542%
56	10.049	1465	1470	1483	rVB	386935	555216	56.98%	7.469%
57	10.305	1506	1512	1521	rBV7	1498	3569	0.37%	0.048%
58	10.561	1553	1554	1562	rVB4	660	776	0.08%	0.010%
59	10.622	1562	1564	1565	rBV2	531	505	0.05%	0.007%
60	10.646	1565	1568	1574	rVV2	4818	6557	0.67%	0.088%
61	10.884	1601	1607	1609	rVB2	974	1652	0.17%	0.022%
62	10.921	1611	1613	1616	rVV2	517	594	0.06%	0.008%
63	10.970	1616	1621	1624	rVV2	650	919	0.09%	0.012%
64	11.006	1624	1627	1628	rBV3	673	641	0.07%	0.009%
65	11.134	1647	1648	1652	rBV3	584	649	0.07%	0.009%
66	11.189	1652	1657	1670	rVV	359380	456450	46.84%	6.140%
67	11.457	1699	1701	1705	rVB4	1032	1081	0.11%	0.015%
68	11.616	1725	1727	1730	rVB3	484	533	0.05%	0.007%
69	11.756	1748	1750	1754	rBV4	1064	1300	0.13%	0.017%
70	11.847	1762	1765	1768	rBV2	474	617	0.06%	0.008%
71	12.018	1788	1793	1803	rBV	393425	498922	51.20%	6.712%
72	12.232	1825	1828	1829	rBV2	731	666	0.07%	0.009%
73	12.317	1836	1842	1856	rBV	561341	706467	72.50%	9.504%
74	12.616	1888	1891	1893	rBV2	550	673	0.07%	0.009%
75	12.664	1897	1899	1901	rBV	676	603	0.06%	0.008%
76	12.695	1902	1904	1906	rVB2	601	488	0.05%	0.007%

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 Title : VOC Analysis

77	12.762	1911	1915	1920	rVB3	2075	3388	0.35%	0.046%
78	12.902	1935	1938	1945	rVB5	1767	2961	0.30%	0.040%
79	13.134	1974	1976	1978	rVB3	600	422	0.04%	0.006%
80	13.158	1978	1980	1981	rBV2	495	398	0.04%	0.005%
81	13.341	2006	2010	2014	rBV5	1354	2255	0.23%	0.030%
82	13.439	2021	2026	2028	rBV3	619	1092	0.11%	0.015%
83	13.652	2059	2061	2065	rBV3	575	888	0.09%	0.012%
84	13.731	2072	2074	2077	rVB2	649	436	0.04%	0.006%
85	13.780	2079	2082	2087	rVV3	1496	2102	0.22%	0.028%
86	14.128	2135	2139	2144	rBV	1981	3612	0.37%	0.049%
87	14.280	2163	2164	2166	rBV2	659	417	0.04%	0.006%
88	14.487	2195	2198	2201	rBV3	384	437	0.04%	0.006%
89	14.542	2205	2207	2209	rBV2	693	448	0.05%	0.006%
90	15.018	2283	2285	2287	rBV2	554	520	0.05%	0.007%
91	15.109	2298	2300	2304	rBV3	585	671	0.07%	0.009%
92	15.170	2308	2310	2314	rVB4	661	624	0.06%	0.008%
93	15.207	2314	2316	2317	rBV2	626	432	0.04%	0.006%
94	15.286	2327	2329	2331	rBV2	766	466	0.05%	0.006%
95	15.383	2343	2345	2349	rBV5	1229	1726	0.18%	0.023%
96	15.597	2379	2380	2382	rBV2	631	409	0.04%	0.006%
97	16.066	2454	2457	2458	rBV2	656	592	0.06%	0.008%
98	16.499	2526	2528	2531	rBV3	636	475	0.05%	0.006%
99	16.603	2543	2545	2547	rBV2	573	492	0.05%	0.007%
100	16.743	2566	2568	2571	rBV3	728	603	0.06%	0.008%

Sum of corrected areas: 7433443

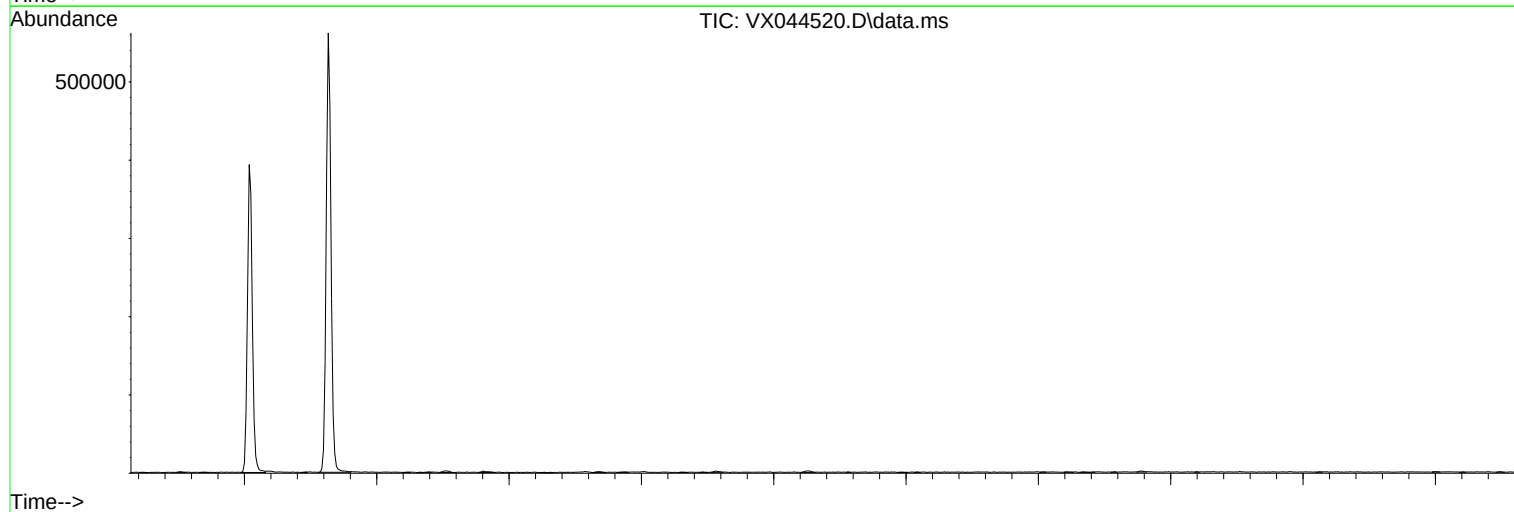
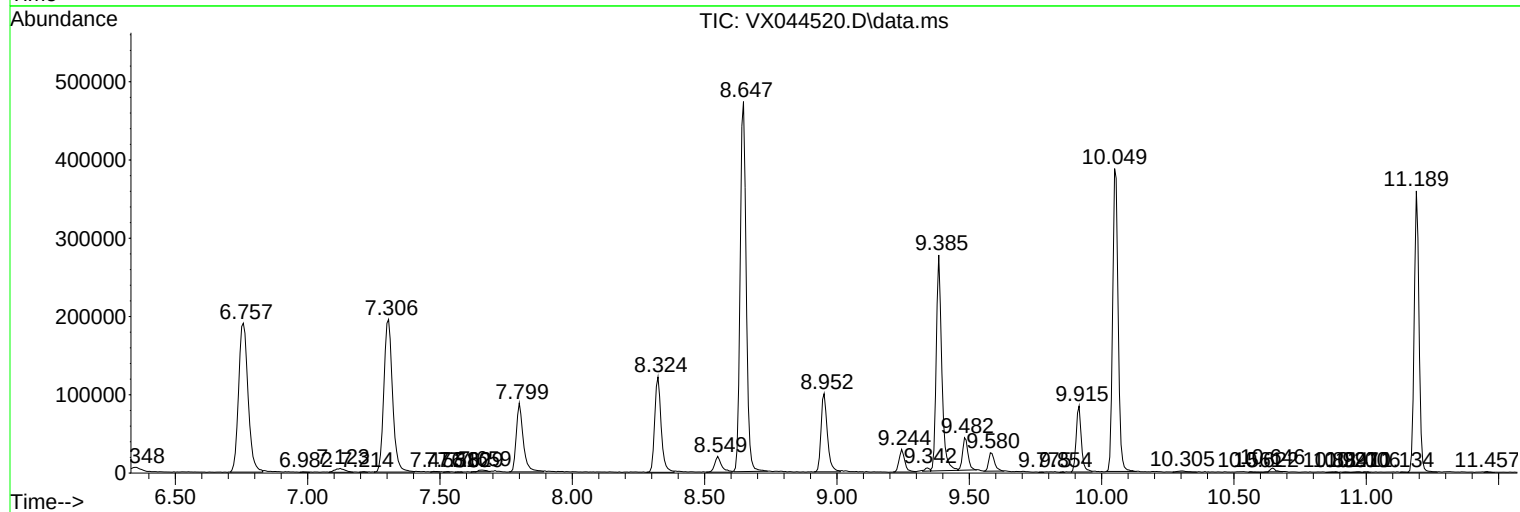
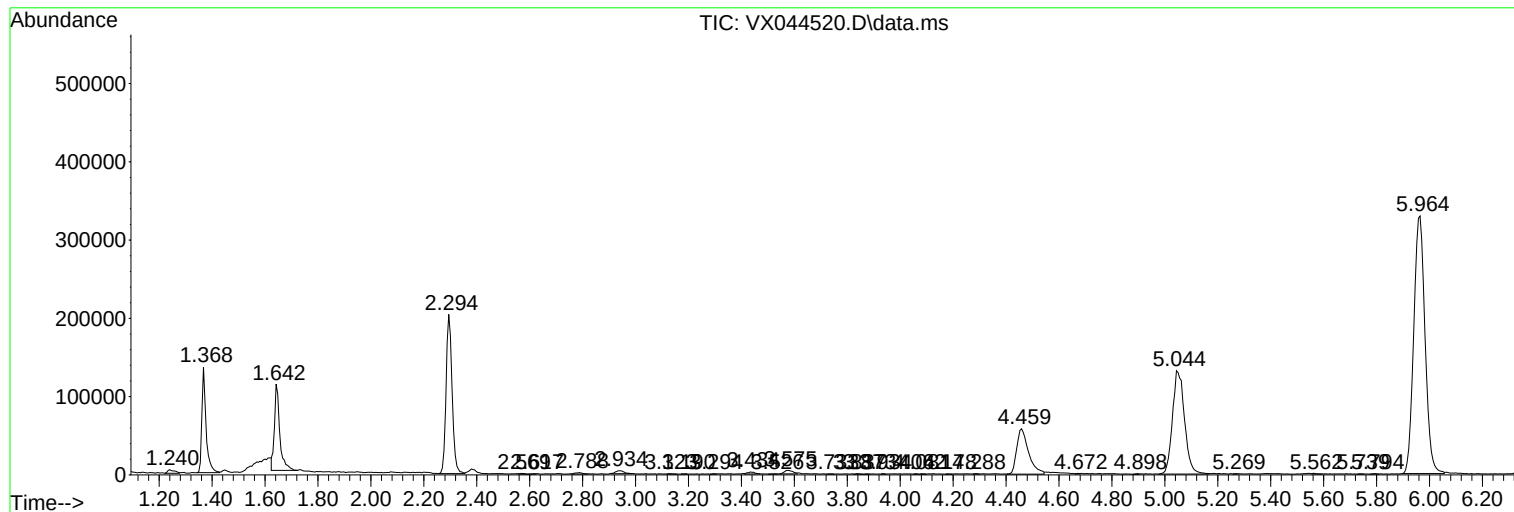
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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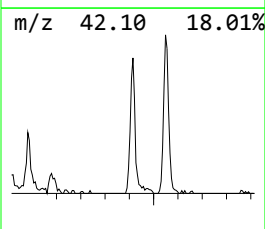
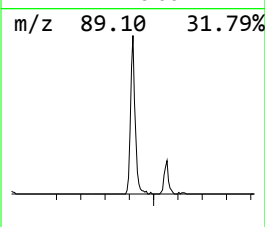
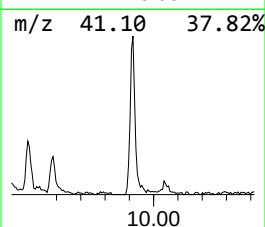
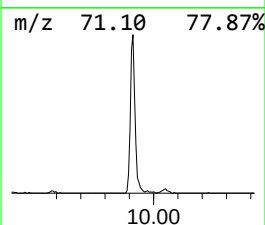
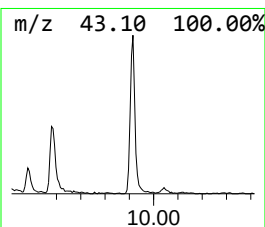
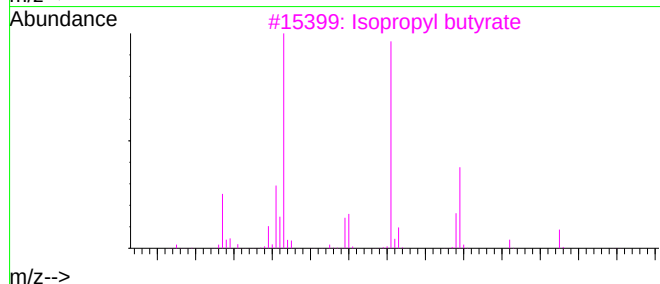
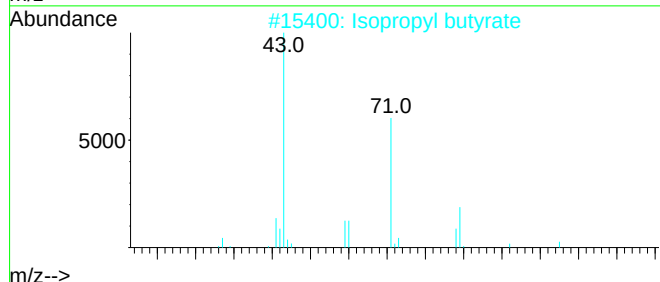
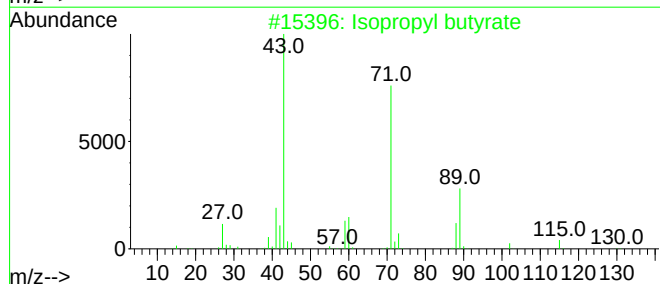
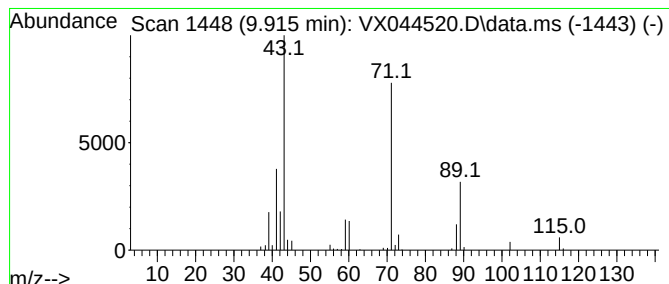
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	10.32 ug/L	114589	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	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64



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TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isopropyl butyrate	9.915	10.3	ug/L	114589	2	10.055	555216	50.0