

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044360.D
 Acq On : 17 Dec 2024 18:37
 Operator : JC/MD
 Sample : P5263-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DCZF0

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: VX044360.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	33	rVB6	3477	6908	0.72%	0.093%
2	1.368	43	46	56	rVB	109253	120034	12.52%	1.613%
3	1.648	88	92	100	rVB	99564	135299	14.12%	1.819%
4	2.294	192	198	210	rBV	174329	277150	28.92%	3.725%
5	2.556	240	241	245	rBV4	927	1003	0.10%	0.013%
6	2.648	253	256	260	rBV2	935	1099	0.11%	0.015%
7	2.782	274	278	285	rBV7	1803	3419	0.36%	0.046%
8	2.947	297	305	310	rVV2	6577	14737	1.54%	0.198%
9	2.989	310	312	315	rVV3	888	860	0.09%	0.012%
10	3.032	317	319	321	rBV2	629	532	0.06%	0.007%
11	3.075	324	326	327	rBV	571	477	0.05%	0.006%
12	3.306	361	364	366	rBV3	402	474	0.05%	0.006%
13	3.428	380	384	385	rBV3	1491	1944	0.20%	0.026%
14	3.587	405	410	415	rBV4	1245	2690	0.28%	0.036%
15	4.026	481	482	485	rVB2	589	616	0.06%	0.008%
16	4.062	485	488	490	rBV	664	716	0.07%	0.010%
17	4.227	514	515	518	rBV2	491	576	0.06%	0.008%
18	4.458	546	553	567	rBV	67636	201768	21.05%	2.712%
19	4.812	607	611	614	rBV5	529	680	0.07%	0.009%
20	4.855	617	618	621	rVB2	707	622	0.06%	0.008%
21	4.897	621	625	626	rBV2	721	876	0.09%	0.012%
22	4.971	634	637	638	rBV2	597	534	0.06%	0.007%
23	5.056	640	651	670	rVB	129601	409129	42.68%	5.499%
24	5.501	722	724	728	rVB3	360	493	0.05%	0.007%
25	5.544	728	731	732	rBV3	767	622	0.06%	0.008%
26	5.964	789	800	817	rVV2	318486	958495	100.00%	12.884%
27	6.178	833	835	839	rBV4	531	847	0.09%	0.011%
28	6.348	857	863	874	rVV3	6424	18074	1.89%	0.243%
29	6.757	919	930	945	rBV	235278	576455	60.14%	7.749%
30	7.056	978	979	982	rBV2	771	646	0.07%	0.009%
31	7.123	984	990	995	rBV7	2531	6397	0.67%	0.086%
32	7.305	1012	1020	1031	rBV	210035	450516	47.00%	6.056%
33	7.665	1072	1079	1080	rBV2	3248	5599	0.58%	0.075%
34	7.799	1095	1101	1115	rBV	89319	167535	17.48%	2.252%
35	8.074	1143	1146	1150	rVB4	557	880	0.09%	0.012%
36	8.324	1181	1187	1199	rVV	119917	196292	20.48%	2.639%

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

37	8.446	1205	1207	1210	rBV3	495	487	0.05%	0.007%
38	8.549	1217	1224	1233	rBV2	19625	34800	3.63%	0.468%
39	8.647	1234	1240	1252	rVV	439832	693845	72.39%	9.327%
40	8.952	1284	1290	1303	rBV2	100658	166881	17.41%	2.243%
41	9.244	1333	1338	1348	rBV	29903	43656	4.55%	0.587%
42	9.317	1348	1350	1351	rBV2	1866	1622	0.17%	0.022%
43	9.342	1352	1354	1356	rVV3	3892	3435	0.36%	0.046%
44	9.384	1356	1361	1373	rVV	304281	451814	47.14%	6.073%
45	9.482	1373	1377	1383	rVV	42666	57323	5.98%	0.771%
46	9.586	1390	1394	1399	rBV	25868	38321	4.00%	0.515%
47	9.799	1426	1429	1435	rVB5	931	1572	0.16%	0.021%
48	9.915	1443	1448	1460	rBV	84061	118281	12.34%	1.590%
49	10.055	1465	1471	1486	rVB	463148	660763	68.94%	8.882%
50	10.238	1499	1501	1503	rBV2	712	674	0.07%	0.009%
51	10.293	1507	1510	1511	rBV3	805	994	0.10%	0.013%
52	10.396	1525	1527	1530	rBV4	586	574	0.06%	0.008%
53	10.451	1533	1536	1538	rBV3	633	805	0.08%	0.011%
54	10.470	1538	1539	1543	rBV2	474	722	0.08%	0.010%
55	10.646	1564	1568	1577	rBV3	4480	7769	0.81%	0.104%
56	10.713	1577	1579	1581	rBV2	586	569	0.06%	0.008%
57	10.817	1594	1596	1600	rVB3	369	547	0.06%	0.007%
58	10.860	1600	1603	1606	rBV2	601	765	0.08%	0.010%
59	10.902	1608	1610	1612	rBV2	685	560	0.06%	0.008%
60	10.933	1612	1615	1619	rBV3	629	818	0.09%	0.011%
61	11.055	1634	1635	1637	rBV2	560	540	0.06%	0.007%
62	11.189	1651	1657	1667	rBV	392367	475488	49.61%	6.391%
63	11.366	1685	1686	1689	rBV2	525	496	0.05%	0.007%
64	11.640	1729	1731	1733	rBV2	495	523	0.05%	0.007%
65	11.738	1743	1747	1748	rBV	851	705	0.07%	0.009%
66	11.902	1772	1774	1775	rBV2	604	580	0.06%	0.008%
67	11.933	1775	1779	1780	rVV2	596	745	0.08%	0.010%
68	12.018	1788	1793	1802	rBV	398171	517171	53.96%	6.952%
69	12.317	1837	1842	1857	rBV	452847	569689	59.44%	7.658%
70	12.433	1860	1861	1864	rVB3	645	556	0.06%	0.007%
71	12.506	1871	1873	1878	rBV4	656	1055	0.11%	0.014%
72	12.640	1893	1895	1896	rBV2	528	494	0.05%	0.007%
73	12.695	1903	1904	1907	rVB	794	567	0.06%	0.008%
74	12.750	1911	1913	1915	rBV2	589	651	0.07%	0.009%
75	12.975	1947	1950	1952	rBV3	612	593	0.06%	0.008%
76	13.219	1989	1990	1992	rBV2	561	470	0.05%	0.006%

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Integration Parameters: LSCINT.P

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Min Area: 0 % of largest Peak

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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

77	13.335	2006	2009	2010	rBV2	505	571	0.06%	0.008%
78	13.365	2013	2014	2018	rVB2	601	545	0.06%	0.007%
79	13.518	2037	2039	2042	rBV3	504	535	0.06%	0.007%
80	13.579	2047	2049	2052	rBV2	402	624	0.07%	0.008%
81	13.670	2061	2064	2065	rBV2	507	509	0.05%	0.007%
82	13.725	2072	2073	2080	rVB2	780	772	0.08%	0.010%
83	13.817	2087	2088	2091	rVB3	717	642	0.07%	0.009%
84	14.018	2116	2121	2122	rBV2	752	848	0.09%	0.011%
85	14.109	2134	2136	2137	rBV2	1048	852	0.09%	0.011%
86	14.152	2142	2143	2145	rBV2	634	574	0.06%	0.008%
87	14.249	2156	2159	2162	rVB3	490	549	0.06%	0.007%
88	14.329	2170	2172	2173	rBV	710	548	0.06%	0.007%
89	14.438	2188	2190	2192	rVB2	821	664	0.07%	0.009%
90	14.774	2242	2245	2246	rBV	591	530	0.06%	0.007%
91	14.889	2263	2264	2268	rBV2	471	654	0.07%	0.009%
92	15.395	2344	2347	2350	rVB4	873	1092	0.11%	0.015%
93	15.566	2373	2375	2378	rBV3	674	942	0.10%	0.013%
94	15.591	2378	2379	2381	rBV2	744	576	0.06%	0.008%
95	15.652	2388	2389	2391	rBV2	839	642	0.07%	0.009%
96	15.694	2394	2396	2397	rBV2	639	596	0.06%	0.008%
97	15.993	2443	2445	2452	rVB3	889	1021	0.11%	0.014%
98	16.347	2501	2503	2504	rBV	522	464	0.05%	0.006%
99	16.444	2518	2519	2523	rVB3	749	710	0.07%	0.010%
100	16.493	2523	2527	2529	rBV2	717	1116	0.12%	0.015%

Sum of corrected areas: 7439490

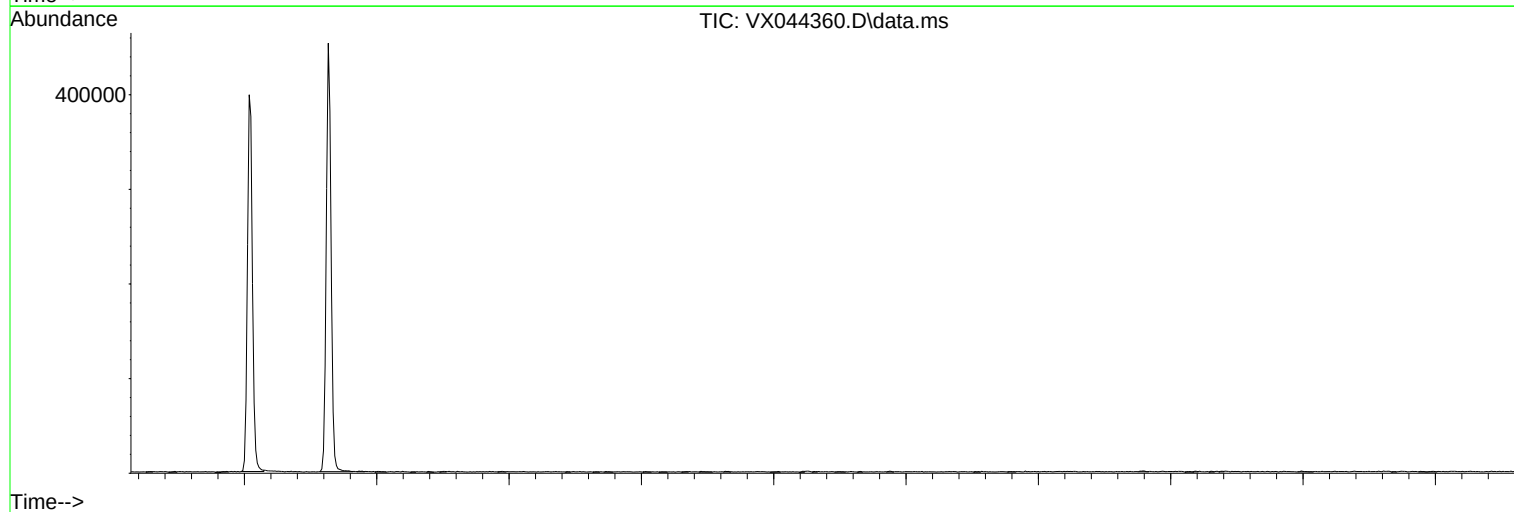
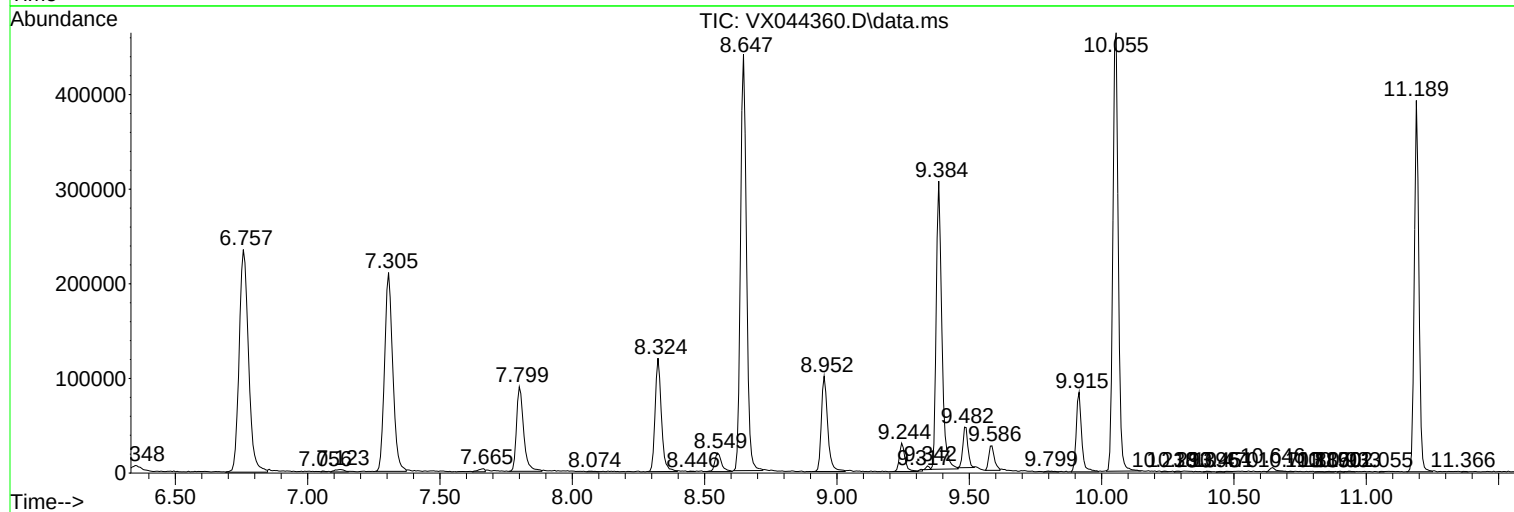
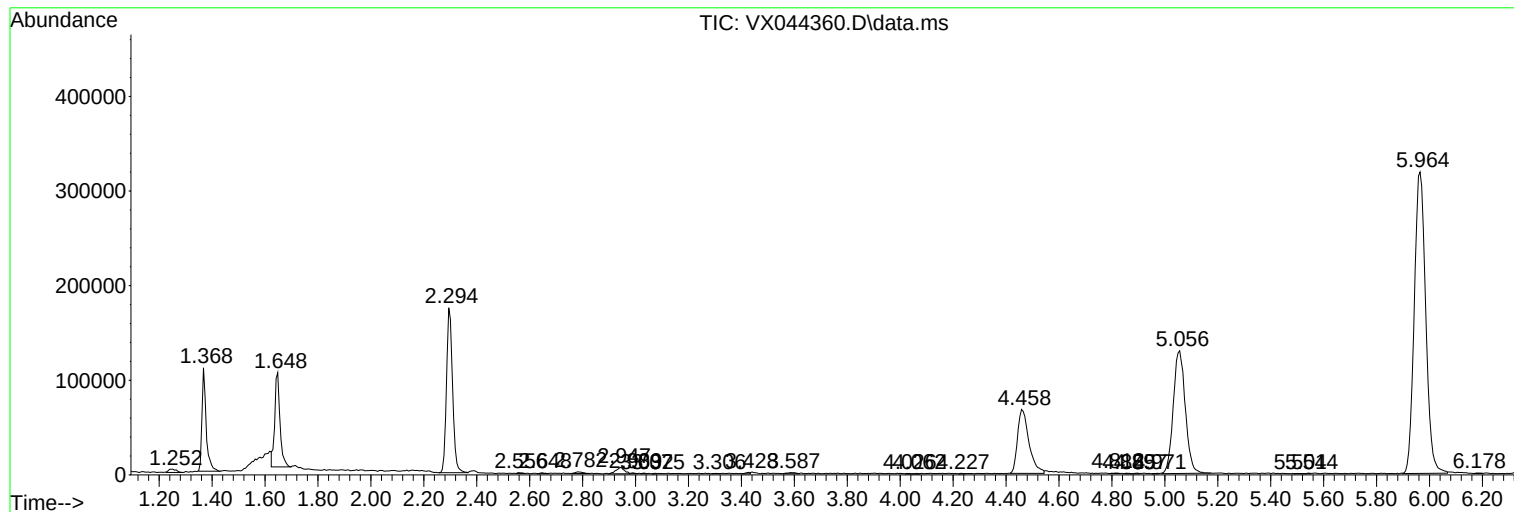
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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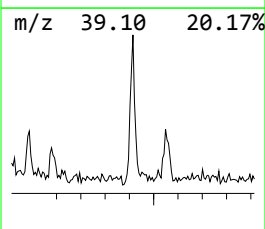
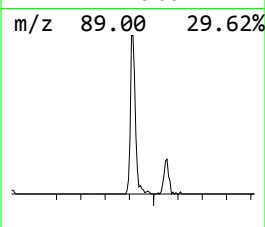
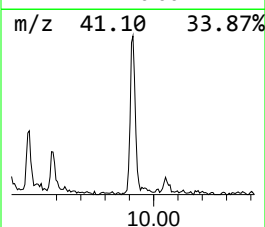
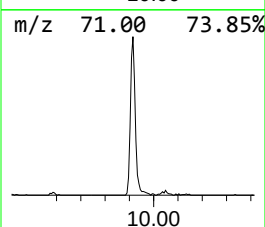
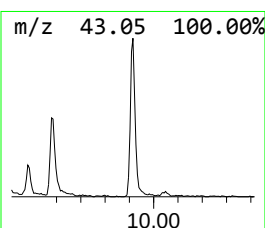
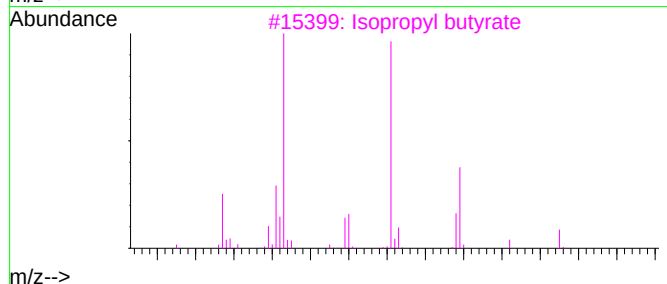
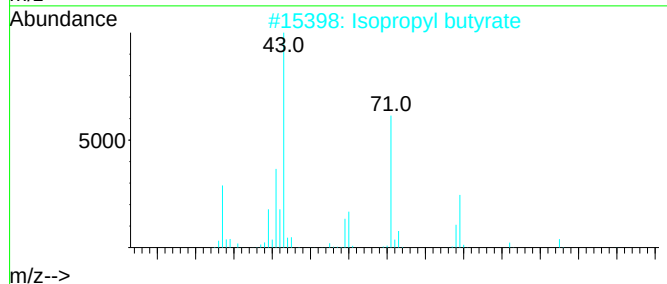
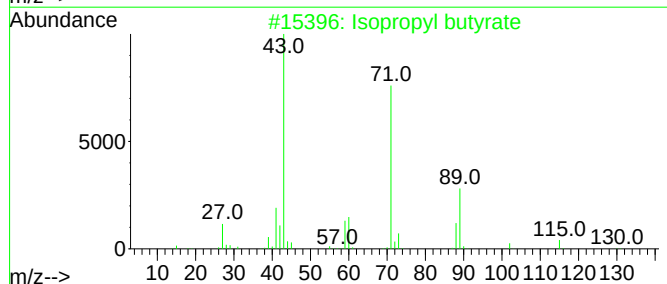
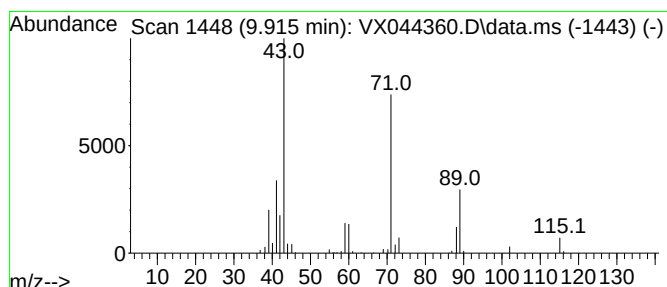
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	8.95 ug/L	118281	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	90
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	78
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
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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	118281	2	10.055	660763	50.0