

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012825\
 Data File : VX044750.D
 Acq On : 28 Jan 2025 17:30
 Operator : JC/MD
 Sample : Q1162-02 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E2947

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\SFAMXML012825WMA.M
 Title : VOC Analysis

Signal : TIC: VX044750.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	21	25	38	rBV	16521	30618	2.81%	0.371%
2	1.368	42	46	61	rVB	130422	158315	14.55%	1.921%
3	1.642	88	91	103	rVB	54108	69318	6.37%	0.841%
4	2.294	192	198	208	rBV	240317	376602	34.62%	4.569%
5	2.386	210	213	221	rVB	6517	11101	1.02%	0.135%
6	2.940	298	304	314	rVB2	6367	15917	1.46%	0.193%
7	3.075	324	326	330	rBV3	398	570	0.05%	0.007%
8	3.123	332	334	336	rBV3	543	405	0.04%	0.005%
9	3.757	436	438	439	rBV	442	253	0.02%	0.003%
10	4.233	515	516	519	rBV2	292	265	0.02%	0.003%
11	4.349	533	535	537	rBV	383	326	0.03%	0.004%
12	4.458	545	553	569	rBV	66503	208518	19.17%	2.530%
13	4.818	610	612	614	rBV2	418	359	0.03%	0.004%
14	5.050	638	650	672	rBV	133268	418140	38.43%	5.073%
15	5.324	692	695	697	rBV	431	564	0.05%	0.007%
16	5.373	701	703	704	rBV	523	402	0.04%	0.005%
17	5.470	717	719	720	rBV2	483	335	0.03%	0.004%
18	5.544	729	731	735	rBV4	656	975	0.09%	0.012%
19	5.647	745	748	750	rBV	314	464	0.04%	0.006%
20	5.720	758	760	763	rVB3	292	311	0.03%	0.004%
21	5.964	789	800	827	rBV2	365576	1087921	100.00%	13.199%
22	6.300	853	855	857	rBV3	509	484	0.04%	0.006%
23	6.348	857	863	873	rVV2	6483	17448	1.60%	0.212%
24	6.684	916	918	919	rBV2	355	322	0.03%	0.004%
25	6.757	921	930	950	rBV	269701	672935	61.86%	8.164%
26	7.123	985	990	992	rBV4	825	1375	0.13%	0.017%
27	7.305	1010	1020	1038	rBV	222488	495749	45.57%	6.015%
28	7.665	1073	1079	1081	rBV	3147	5618	0.52%	0.068%
29	7.799	1096	1101	1112	rBV	61210	116780	10.73%	1.417%
30	8.129	1153	1155	1157	rBV3	445	472	0.04%	0.006%
31	8.324	1181	1187	1198	rBV	155248	265014	24.36%	3.215%
32	8.549	1219	1224	1233	rBV	21381	35911	3.30%	0.436%
33	8.647	1234	1240	1263	rVB	508468	856845	78.76%	10.395%
34	8.945	1284	1289	1303	rBV2	113608	190965	17.55%	2.317%
35	9.134	1318	1320	1321	rVB2	566	307	0.03%	0.004%
36	9.244	1331	1338	1346	rBV	35610	51283	4.71%	0.622%

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 Title : VOC Analysis

37	9.384	1356	1361	1374	rBV2	259119	400609	36.82%	4.860%
38	9.482	1374	1377	1388	rVB	34531	52803	4.85%	0.641%
39	9.586	1390	1394	1403	rVB2	10120	17130	1.57%	0.208%
40	9.872	1440	1441	1442	rBV	459	246	0.02%	0.003%
41	9.909	1442	1447	1457	rVV	81900	117087	10.76%	1.421%
42	10.049	1465	1470	1490	rBV	515287	782804	71.95%	9.497%
43	10.451	1534	1536	1539	rBV	394	289	0.03%	0.004%
44	10.531	1544	1549	1550	rBV3	577	1040	0.10%	0.013%
45	10.652	1564	1569	1573	rBV2	2722	4473	0.41%	0.054%
46	10.878	1603	1606	1609	rBV2	357	535	0.05%	0.006%
47	11.012	1625	1628	1629	rVB	543	523	0.05%	0.006%
48	11.037	1629	1632	1633	rBV	541	707	0.06%	0.009%
49	11.067	1635	1637	1638	rVV2	381	335	0.03%	0.004%
50	11.085	1638	1640	1641	rVV	587	331	0.03%	0.004%
51	11.110	1642	1644	1647	rVV2	532	434	0.04%	0.005%
52	11.140	1647	1649	1652	rVV2	395	475	0.04%	0.006%
53	11.189	1652	1657	1670	rVB	379403	482787	44.38%	5.857%
54	11.457	1693	1701	1703	rBV	555	1202	0.11%	0.015%
55	11.506	1708	1709	1712	rVB2	386	315	0.03%	0.004%
56	11.561	1716	1718	1719	rBV2	316	273	0.03%	0.003%
57	11.701	1739	1741	1746	rVB2	797	992	0.09%	0.012%
58	11.756	1746	1750	1753	rBV2	653	1025	0.09%	0.012%
59	11.908	1773	1775	1780	rVB2	468	658	0.06%	0.008%
60	11.975	1780	1786	1788	rBV2	848	1256	0.12%	0.015%
61	12.018	1788	1793	1807	rVV	491303	630471	57.95%	7.649%
62	12.213	1824	1825	1827	rBV2	532	379	0.03%	0.005%
63	12.317	1837	1842	1856	rBV	511737	629186	57.83%	7.633%
64	12.512	1872	1874	1875	rBV2	450	329	0.03%	0.004%
65	12.713	1905	1907	1909	rVB2	496	349	0.03%	0.004%
66	12.762	1911	1915	1918	rBV3	816	1311	0.12%	0.016%
67	12.847	1926	1929	1930	rBV	452	544	0.05%	0.007%
68	13.079	1963	1967	1970	rBV2	451	469	0.04%	0.006%
69	13.170	1981	1982	1985	rVB2	319	331	0.03%	0.004%
70	13.341	2006	2010	2011	rBV2	412	358	0.03%	0.004%
71	13.365	2012	2014	2017	rVV2	433	403	0.04%	0.005%
72	13.396	2017	2019	2024	rVB	313	300	0.03%	0.004%
73	13.463	2028	2030	2033	rVB2	442	331	0.03%	0.004%
74	13.567	2045	2047	2048	rBV	404	332	0.03%	0.004%
75	13.713	2067	2071	2072	rBV2	398	425	0.04%	0.005%
76	13.731	2072	2074	2077	rBV2	392	461	0.04%	0.006%

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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\SFAMXML012825WMA.M
 Title : VOC Analysis

77	13.768	2079	2080	2082	rBV	362	326	0.03%	0.004%
78	13.792	2082	2084	2088	rVV2	694	1059	0.10%	0.013%
79	13.829	2088	2090	2096	rVB	672	987	0.09%	0.012%
80	13.914	2102	2104	2106	rVB2	555	390	0.04%	0.005%
81	13.938	2106	2108	2111	rBV	338	518	0.05%	0.006%
82	14.018	2119	2121	2125	rBV3	504	797	0.07%	0.010%
83	14.073	2127	2130	2134	rBV3	447	653	0.06%	0.008%
84	14.134	2136	2140	2143	rVV4	1350	1862	0.17%	0.023%
85	14.243	2156	2158	2160	rBV2	287	258	0.02%	0.003%
86	14.444	2190	2191	2194	rVB3	757	718	0.07%	0.009%
87	14.707	2232	2234	2236	rBV2	493	530	0.05%	0.006%
88	14.780	2245	2246	2249	rBV2	392	401	0.04%	0.005%
89	14.804	2249	2250	2252	rVV	398	291	0.03%	0.004%
90	14.829	2252	2254	2255	rVV	376	257	0.02%	0.003%
91	14.981	2278	2279	2280	rBV	495	264	0.02%	0.003%
92	15.133	2303	2304	2310	rVB3	568	617	0.06%	0.007%
93	15.225	2317	2319	2320	rBV	617	388	0.04%	0.005%
94	15.389	2343	2346	2352	rVB4	1068	1687	0.16%	0.020%
95	15.554	2371	2373	2375	rVB2	836	589	0.05%	0.007%
96	15.633	2384	2386	2387	rBV2	610	291	0.03%	0.004%
97	15.682	2392	2394	2395	rBV	776	364	0.03%	0.004%
98	16.066	2455	2457	2460	rBV3	633	855	0.08%	0.010%
99	16.670	2554	2556	2559	rBV4	523	496	0.05%	0.006%
100	16.700	2559	2561	2562	rBV2	629	465	0.04%	0.006%

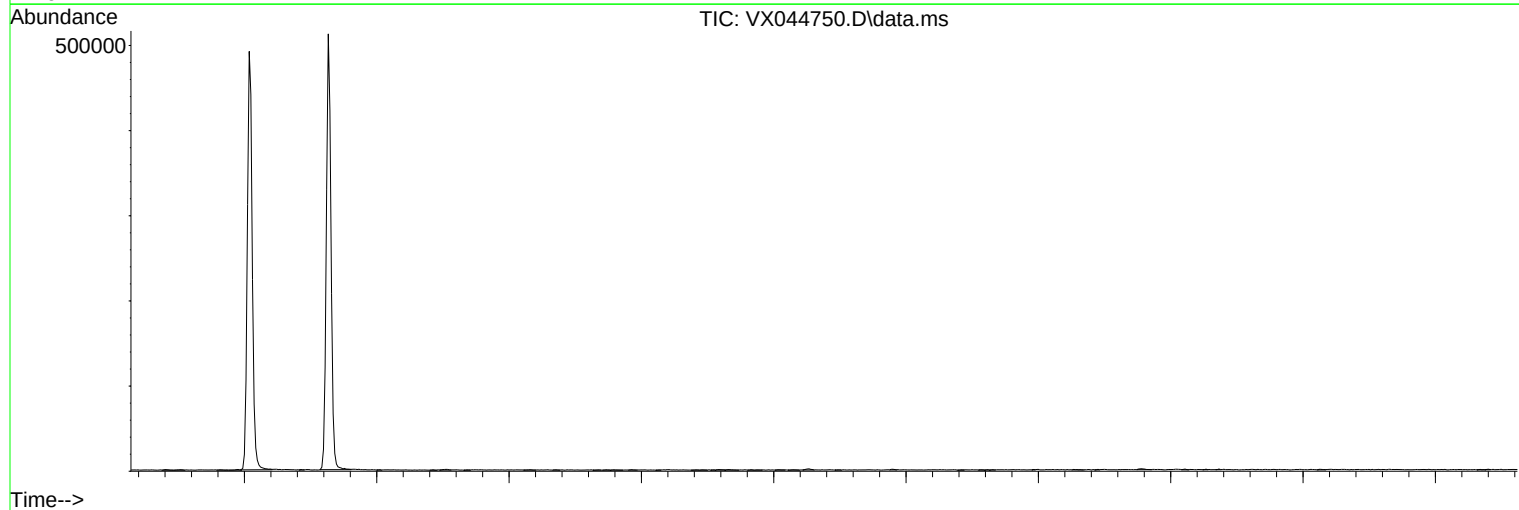
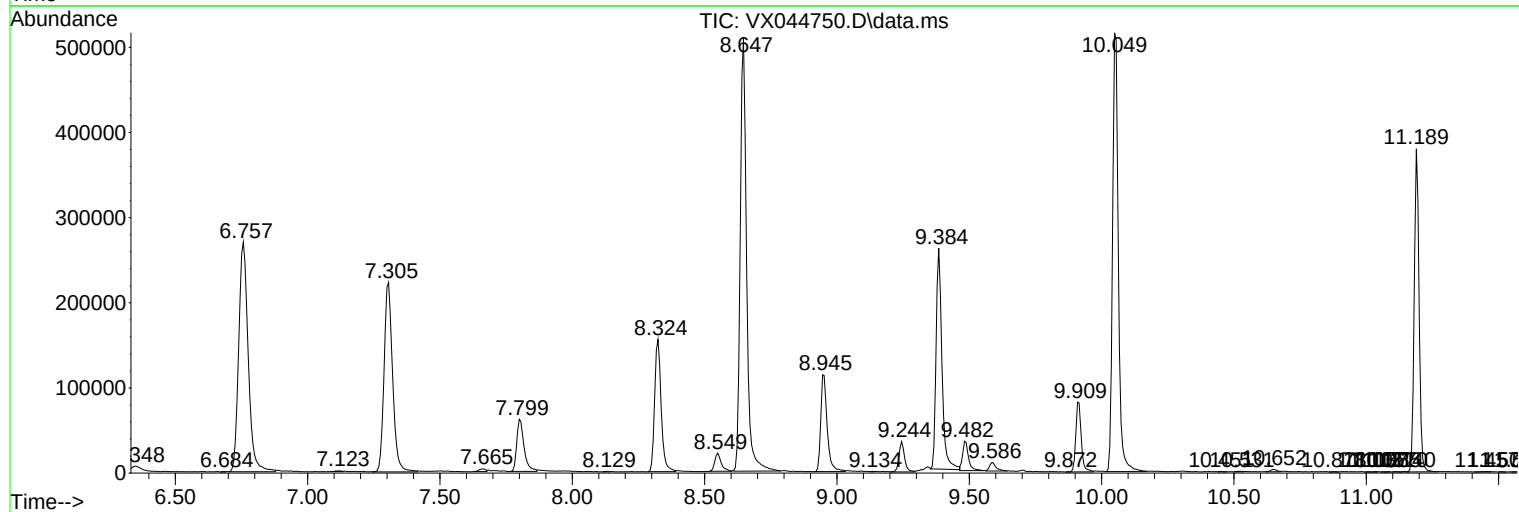
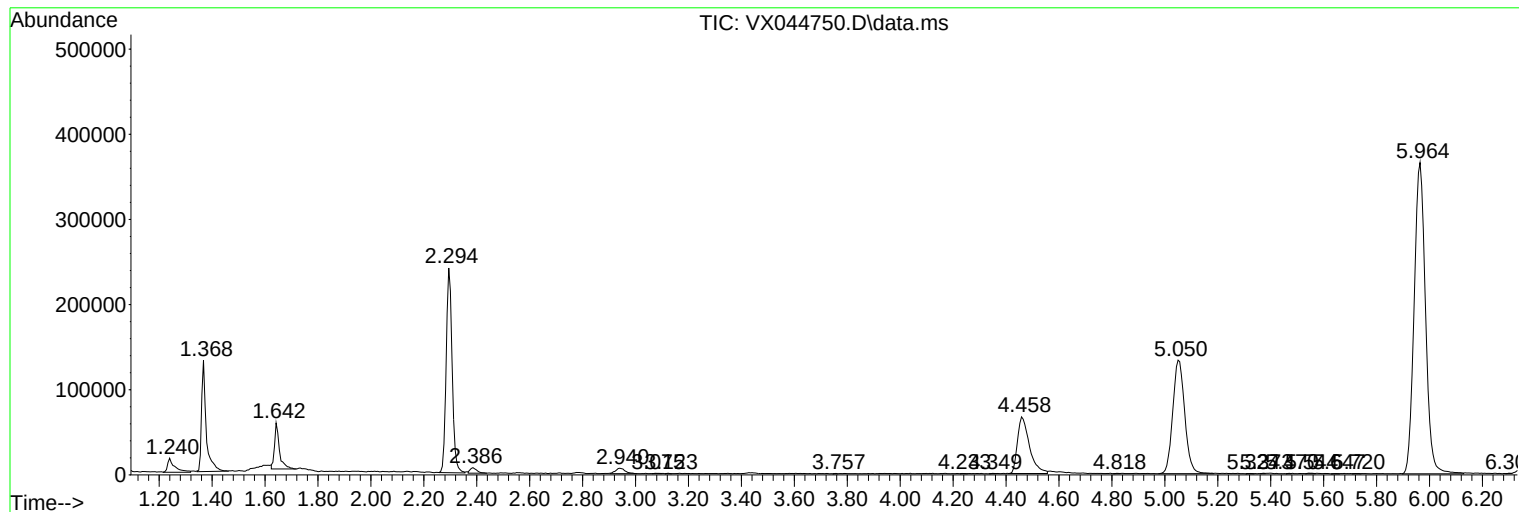
Sum of corrected areas: 8242558

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

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



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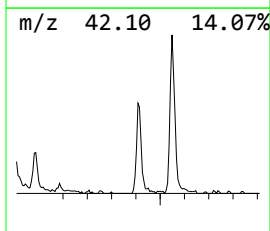
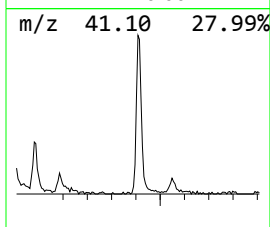
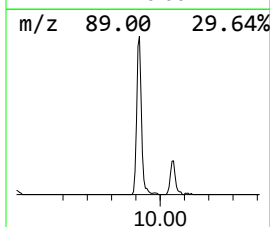
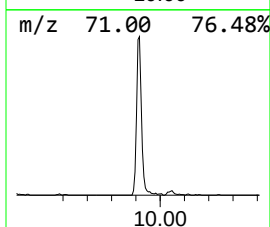
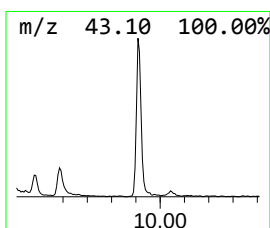
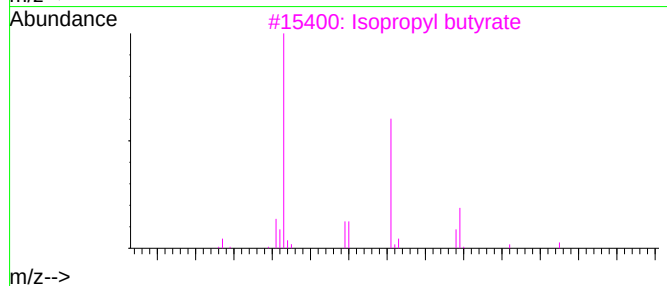
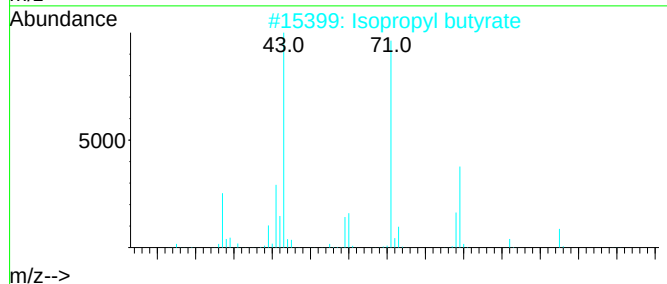
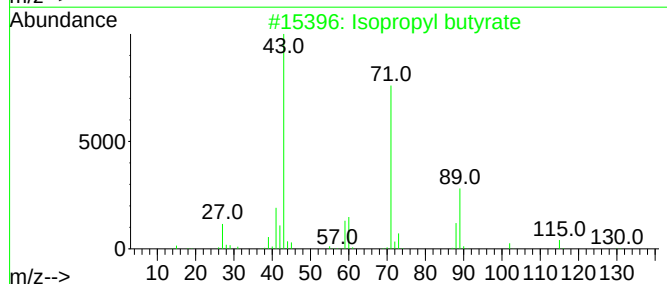
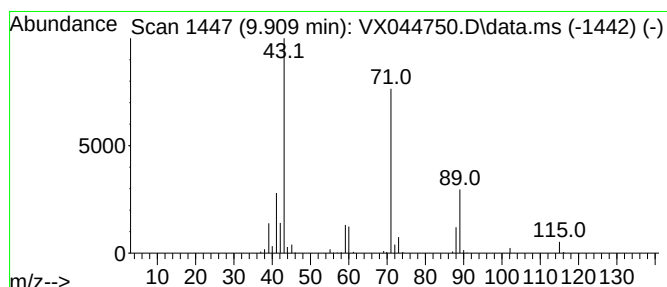
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

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.
9.909	7.48 ug/L	117087	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	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
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	#	RT	Resp	Conc
Isopropyl butyrate	9.909	7.5	ug/L	117087	2	10.055	782804	50.0