

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070224\
 Data File : VU059736.D
 Acq On : 02 Jul 2024 13:58
 Operator : MD/SY
 Sample : P3108-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0ST9

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

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_U\Method\SFAMULM070224WMA.M
 Title : VOC Analysis

Signal : TIC: VU059736.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.518	67	71	77	rBV3	1837	1748	0.17%	0.021%
2	1.596	87	95	114	rBV	124815	148353	14.85%	1.766%
3	1.727	132	136	139	rBV	2629	2484	0.25%	0.030%
4	1.760	143	146	159	rVB2	5760	7395	0.74%	0.088%
5	1.907	183	192	210	rBV	96980	134981	13.51%	1.607%
6	2.560	383	395	410	rBV	209094	337057	33.73%	4.012%
7	2.740	440	451	480	rBV	250929	478900	47.93%	5.700%
8	3.036	538	543	554	rVB5	2423	4167	0.42%	0.050%
9	3.113	564	567	570	rBV2	390	260	0.03%	0.003%
10	3.178	572	587	607	rVB	23407	55733	5.58%	0.663%
11	3.264	610	614	615	rBV	401	244	0.02%	0.003%
12	3.409	655	659	663	rBV3	250	257	0.03%	0.003%
13	3.473	677	679	684	rVB	383	230	0.02%	0.003%
14	3.512	689	691	698	rVB2	321	287	0.03%	0.003%
15	3.554	698	704	707	rBV2	393	438	0.04%	0.005%
16	3.608	717	721	725	rVB	290	220	0.02%	0.003%
17	3.914	814	816	821	rVB2	296	228	0.02%	0.003%
18	4.612	1019	1033	1070	rBV2	103886	270043	27.03%	3.214%
19	4.907	1121	1125	1129	rVB2	598	467	0.05%	0.006%
20	5.052	1154	1170	1198	rBV	174935	396853	39.72%	4.723%
21	5.181	1207	1210	1216	rVB4	767	837	0.08%	0.010%
22	5.213	1216	1220	1222	rVB2	635	512	0.05%	0.006%
23	5.232	1222	1226	1229	rBV3	443	442	0.04%	0.005%
24	5.248	1229	1231	1236	rVB3	505	391	0.04%	0.005%
25	5.300	1242	1247	1251	rBV3	506	505	0.05%	0.006%
26	5.322	1251	1254	1257	rVV2	437	237	0.02%	0.003%
27	5.425	1279	1286	1289	rVB2	343	399	0.04%	0.005%
28	5.612	1333	1344	1350	rBV2	243	506	0.05%	0.006%
29	5.644	1350	1354	1357	rVB	264	257	0.03%	0.003%
30	5.718	1357	1377	1411	rBV2	366163	999147	100.00%	11.892%
31	5.943	1444	1447	1452	rVB3	366	269	0.03%	0.003%
32	6.007	1464	1467	1471	rVB2	290	221	0.02%	0.003%
33	6.049	1477	1480	1484	rVB3	309	216	0.02%	0.003%
34	6.242	1526	1540	1565	rBV	330287	640240	64.08%	7.620%
35	6.534	1622	1631	1632	rBV3	1144	1278	0.13%	0.015%
36	6.682	1661	1677	1706	rBV	222048	439591	44.00%	5.232%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

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_U\Method\SFAMULM070224WMA.M
 Title : VOC Analysis

37	6.795	1710	1712	1718	rVB2	431	311	0.03%	0.004%
38	6.949	1752	1760	1766	rVB2	215	232	0.02%	0.003%
39	7.010	1773	1779	1780	rBV	291	272	0.03%	0.003%
40	7.026	1780	1784	1791	rVB2	325	362	0.04%	0.004%
41	7.074	1794	1799	1804	rBV2	280	283	0.03%	0.003%
42	7.190	1832	1835	1840	rBV2	404	371	0.04%	0.004%
43	7.251	1849	1854	1856	rBV2	194	224	0.02%	0.003%
44	7.560	1931	1950	1973	rBV	119838	217674	21.79%	2.591%
45	7.705	1991	1995	1996	rBV2	484	306	0.03%	0.004%
46	7.824	2028	2032	2040	rBV2	272	373	0.04%	0.004%
47	7.891	2040	2053	2072	rBV	462047	795381	79.61%	9.466%
48	8.174	2130	2141	2162	rBV	81657	143365	14.35%	1.706%
49	8.467	2227	2232	2238	rBV2	1056	1183	0.12%	0.014%
50	8.557	2253	2260	2265	rVB4	953	1251	0.13%	0.015%
51	8.624	2269	2281	2313	rBV	253823	472250	47.27%	5.621%
52	8.878	2357	2360	2363	rBV3	326	295	0.03%	0.004%
53	9.174	2449	2452	2457	rBV2	213	249	0.02%	0.003%
54	9.229	2463	2469	2473	rBV2	221	246	0.02%	0.003%
55	9.412	2513	2526	2556	rBV	473604	801495	80.22%	9.539%
56	9.566	2570	2574	2588	rVB3	1242	1712	0.17%	0.020%
57	9.692	2607	2613	2625	rVB5	1596	2754	0.28%	0.033%
58	9.949	2691	2693	2699	rBV	255	267	0.03%	0.003%
59	9.994	2704	2707	2711	rBV2	231	226	0.02%	0.003%
60	10.036	2717	2720	2723	rBV2	310	250	0.03%	0.003%
61	10.097	2735	2739	2744	rBV3	552	609	0.06%	0.007%
62	10.235	2780	2782	2787	rBV2	250	244	0.02%	0.003%
63	10.492	2857	2862	2866	rVB3	359	346	0.03%	0.004%
64	10.750	2929	2942	2962	rVV	330033	537396	53.79%	6.396%
65	10.891	2979	2986	2992	rVB3	1700	2592	0.26%	0.031%
66	10.936	2997	3000	3004	rBV2	264	217	0.02%	0.003%
67	11.081	3041	3045	3047	rBV	460	296	0.03%	0.004%
68	11.225	3086	3090	3093	rBV	288	298	0.03%	0.004%
69	11.463	3157	3164	3171	rBV3	733	976	0.10%	0.012%
70	11.746	3246	3252	3259	rBV4	1655	2754	0.28%	0.033%
71	11.807	3259	3271	3297	rBV	432040	721815	72.24%	8.591%
72	12.077	3346	3355	3359	rBV5	2960	4885	0.49%	0.058%
73	12.187	3376	3389	3412	rBV	425806	727266	72.79%	8.656%
74	12.389	3446	3452	3457	rBV3	393	476	0.05%	0.006%
75	12.418	3457	3461	3463	rBV2	396	340	0.03%	0.004%
76	12.579	3505	3511	3514	rBV	400	486	0.05%	0.006%

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ClientSampleId :
C0ST9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 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_U\Method\SFAMULM070224WMA.M
Title : VOC Analysis

77	12.663	3533	3537	3540	rBV	316	231	0.02%	0.003%
78	12.955	3625	3628	3633	rVB	303	250	0.03%	0.003%
79	13.052	3654	3658	3662	rBV2	296	332	0.03%	0.004%
80	13.216	3705	3709	3710	rBV2	409	253	0.03%	0.003%
81	13.235	3710	3715	3720	rVV5	619	826	0.08%	0.010%
82	13.312	3735	3739	3741	rBV2	367	316	0.03%	0.004%
83	13.762	3876	3879	3885	rVB2	380	399	0.04%	0.005%
84	13.794	3885	3889	3892	rBV2	344	315	0.03%	0.004%
85	13.843	3895	3904	3919	rVB4	8478	13521	1.35%	0.161%
86	13.904	3919	3923	3927	rBV	379	308	0.03%	0.004%
87	13.942	3933	3935	3938	rVB3	437	245	0.02%	0.003%
88	14.110	3977	3987	3993	rBV2	1014	1767	0.18%	0.021%
89	14.138	3993	3996	4004	rVB3	867	1050	0.11%	0.012%
90	14.331	4048	4056	4069	rVB6	5225	8613	0.86%	0.103%
91	14.576	4128	4132	4134	rBV	388	363	0.04%	0.004%
92	14.630	4146	4149	4153	rBV	509	520	0.05%	0.006%
93	14.704	4169	4172	4173	rBV	307	221	0.02%	0.003%
94	14.733	4178	4181	4183	rBV3	388	240	0.02%	0.003%
95	14.749	4183	4186	4188	rBV2	489	329	0.03%	0.004%
96	15.019	4267	4270	4271	rBV2	410	217	0.02%	0.003%
97	15.618	4452	4456	4459	rBV2	562	493	0.05%	0.006%
98	15.659	4465	4469	4471	rBV2	725	547	0.05%	0.007%
99	16.000	4572	4575	4584	rVB5	2096	2271	0.23%	0.027%
100	16.380	4690	4693	4695	rBV2	1101	786	0.08%	0.009%

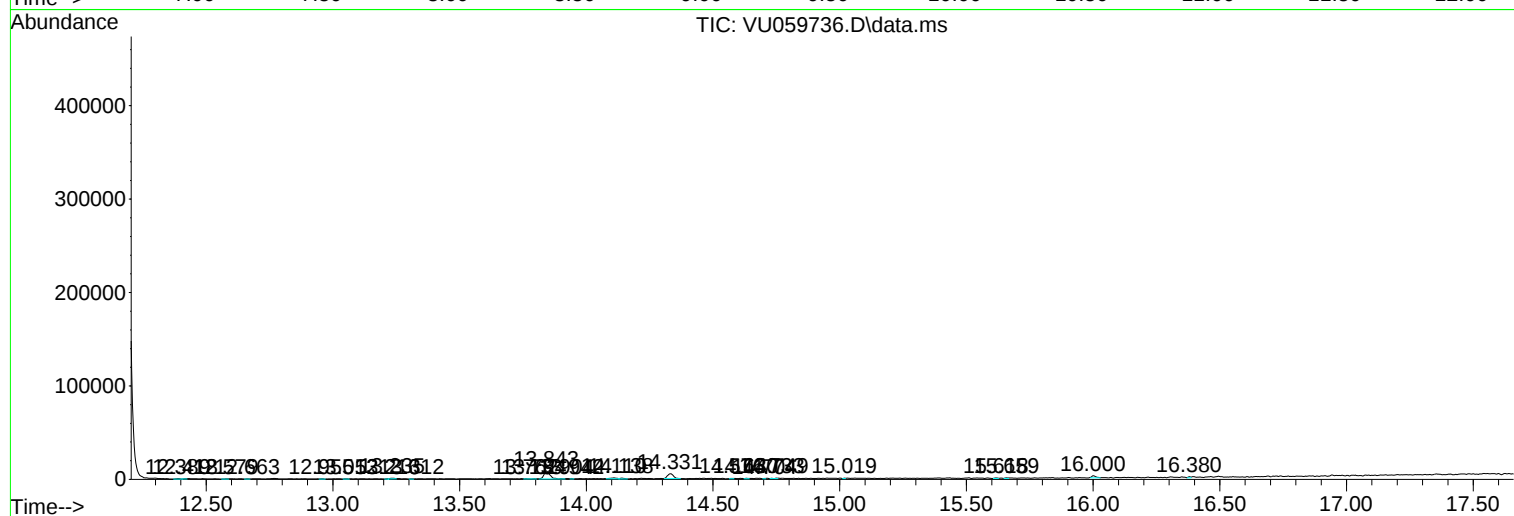
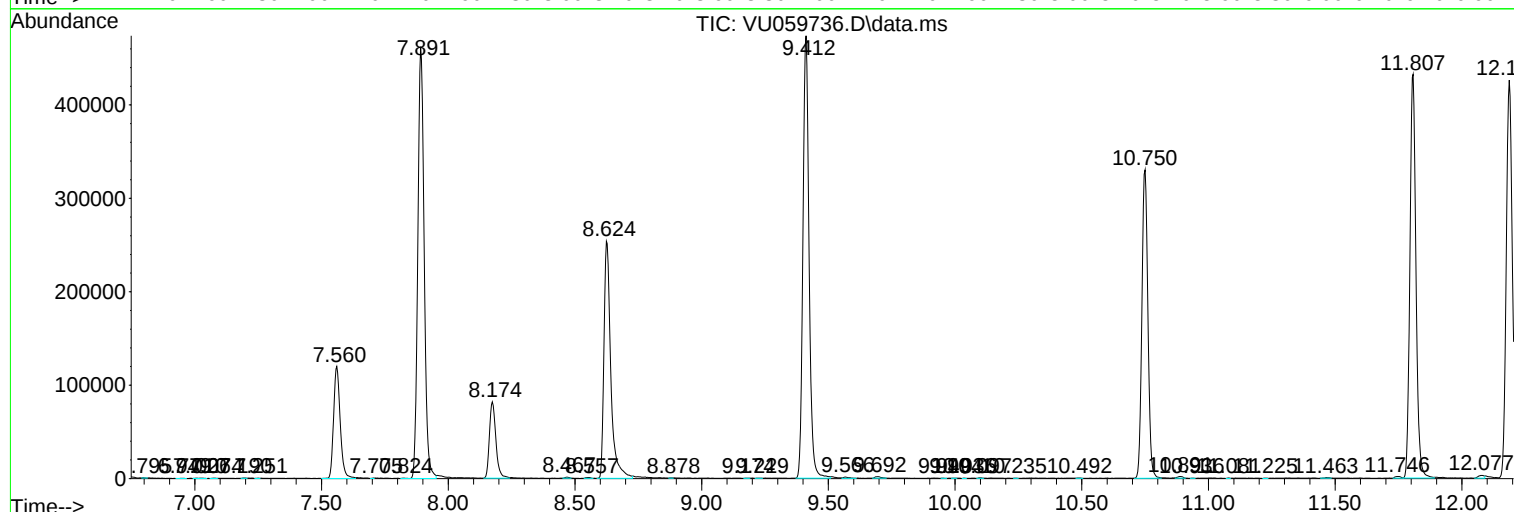
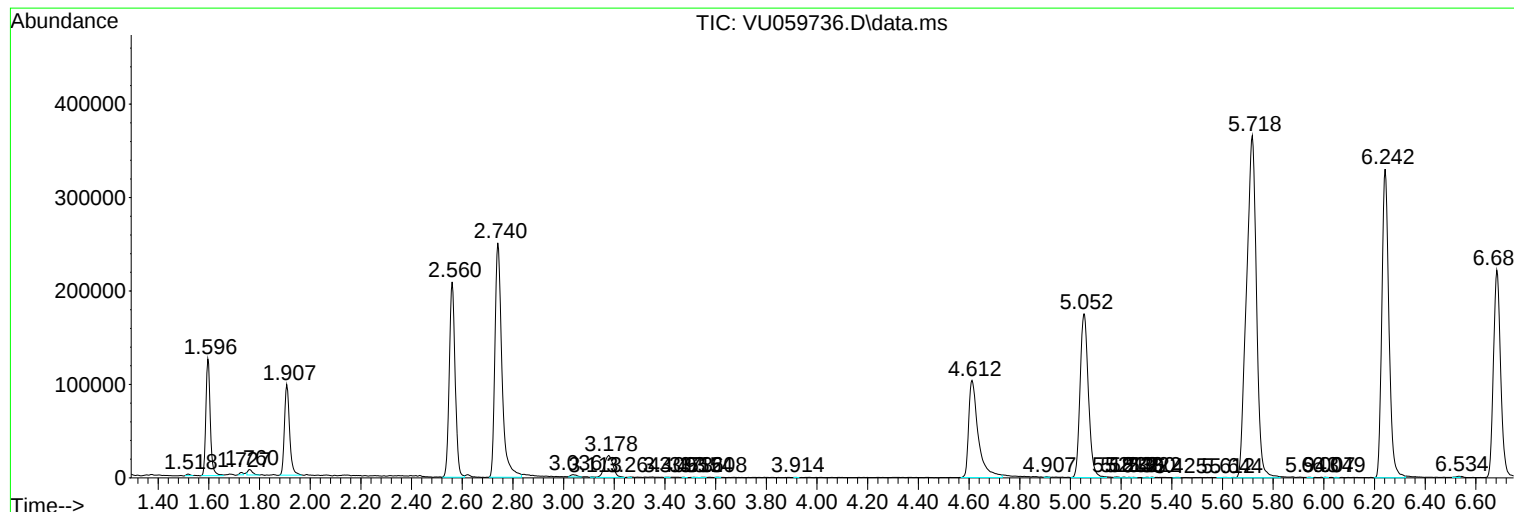
Sum of corrected areas: 8402134

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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



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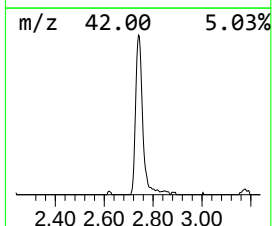
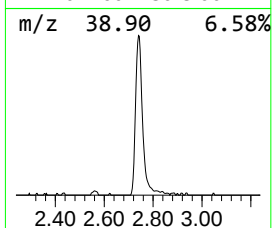
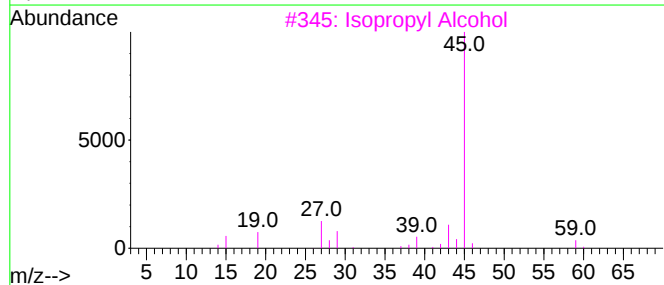
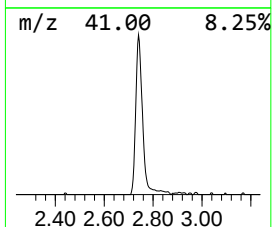
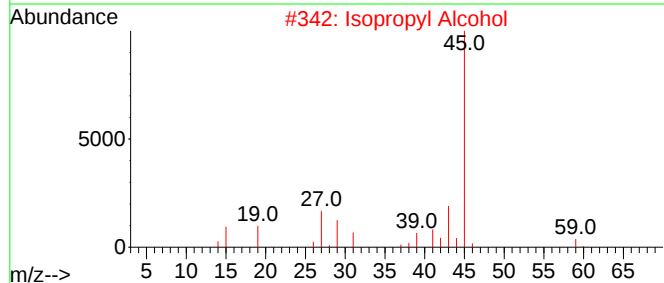
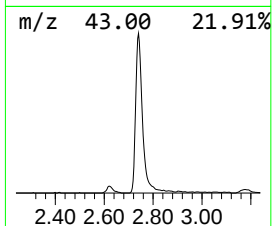
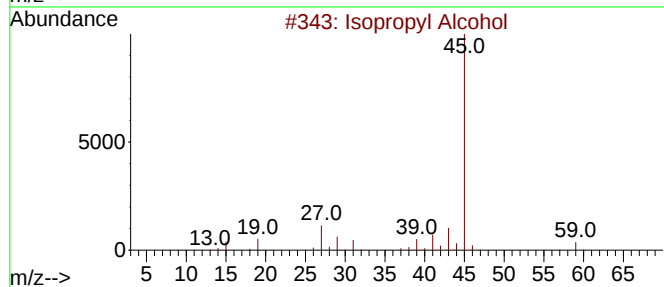
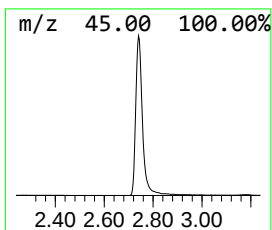
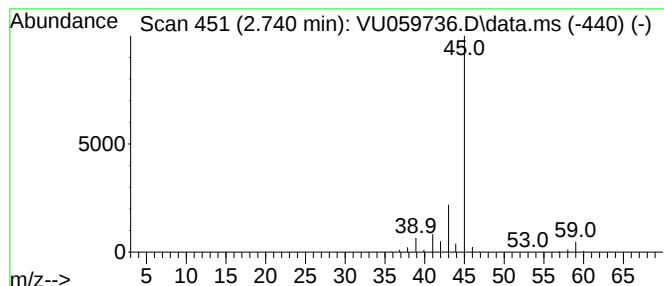
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.740	37.40 ug/L	478900	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol			60	C3H8O	000067-63-0	86
2	Isopropyl Alcohol			60	C3H8O	000067-63-0	78
3	Isopropyl Alcohol			60	C3H8O	000067-63-0	64
4	Isopropyl Alcohol			60	C3H8O	000067-63-0	56
5	Isopropyl Alcohol			60	C3H8O	000067-63-0	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.740	37.4	ug/L	478900	1	6.242	640240	50.0