

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046137.D
 Acq On : 07 Dec 2021 13:55
 Operator : SY/MD
 Sample : M4960-07
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

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\SFAMULM112921WMA.M

Title : VOC Analysis

Signal : TIC: VU046137.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	96	rBV	131420	145496	15.32%	1.996%
2	1.919	171	180	194	rVB	90108	115662	12.18%	1.587%
3	2.340	308	311	315	rBV2	234	182	0.02%	0.002%
4	2.527	366	369	371	rBV2	139	121	0.01%	0.002%
5	2.572	371	383	398	rBV	213586	354160	37.28%	4.859%
6	2.755	435	440	442	rBV	187	197	0.02%	0.003%
7	2.871	473	476	477	rBV	260	147	0.02%	0.002%
8	3.057	528	534	537	rVB2	449	400	0.04%	0.005%
9	3.195	565	577	587	rBV	1946	4460	0.47%	0.061%
10	3.266	596	599	603	rBV	232	243	0.03%	0.003%
11	3.353	623	626	630	rVB	181	132	0.01%	0.002%
12	3.957	811	814	816	rBV2	206	147	0.02%	0.002%
13	4.128	864	867	869	rBV	194	161	0.02%	0.002%
14	4.163	875	878	882	rVB	170	165	0.02%	0.002%
15	4.186	882	885	887	rBV	259	174	0.02%	0.002%
16	4.363	934	940	948	rBB	214	402	0.04%	0.006%
17	4.398	948	951	953	rBV	136	115	0.01%	0.002%
18	4.414	953	956	960	rVB	164	168	0.02%	0.002%
19	4.436	960	963	968	rBB	121	130	0.01%	0.002%
20	4.472	969	974	976	rBV	286	243	0.03%	0.003%
21	4.504	981	984	987	rVV	196	108	0.01%	0.001%
22	4.639	1009	1026	1061	rBV	80357	236517	24.90%	3.245%
23	4.809	1067	1079	1099	rVB4	16673	38724	4.08%	0.531%
24	4.980	1129	1132	1135	rBV	175	175	0.02%	0.002%
25	5.067	1142	1159	1180	rVV	162591	364490	38.37%	5.001%
26	5.289	1222	1228	1235	rBB4	404	614	0.06%	0.008%
27	5.324	1235	1239	1242	rBV	139	162	0.02%	0.002%
28	5.427	1266	1271	1273	rBV	182	208	0.02%	0.003%
29	5.453	1277	1279	1285	rVB	159	111	0.01%	0.002%
30	5.729	1342	1365	1387	rBV2	354009	949966	100.00%	13.033%
31	6.041	1457	1462	1464	rBV4	499	447	0.05%	0.006%
32	6.250	1512	1527	1546	rBV	249932	472161	49.70%	6.478%
33	6.430	1581	1583	1587	rBV2	120	111	0.01%	0.002%
34	6.530	1606	1614	1625	rBV3	4543	8404	0.88%	0.115%
35	6.694	1650	1665	1687	rBV	211322	410785	43.24%	5.636%
36	7.034	1768	1771	1773	rBV2	205	170	0.02%	0.002%

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Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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\SFAMULM112921WMA.M
 Title : VOC Analysis

37	7.086	1783	1787	1794	rVB	148	138	0.01%	0.002%
38	7.186	1812	1818	1825	rVB2	261	364	0.04%	0.005%
39	7.401	1878	1885	1889	rBV	231	193	0.02%	0.003%
40	7.568	1921	1937	1961	rBV	124278	216593	22.80%	2.971%
41	7.684	1970	1973	1977	rVB2	449	314	0.03%	0.004%
42	7.726	1980	1986	1988	rBV2	138	109	0.01%	0.001%
43	7.899	2023	2040	2056	rBV	465387	801562	84.38%	10.997%
44	8.179	2115	2127	2142	rBV	84287	140086	14.75%	1.922%
45	8.253	2149	2150	2159	rVB3	444	511	0.05%	0.007%
46	8.295	2159	2163	2166	rVB2	250	194	0.02%	0.003%
47	8.317	2167	2170	2173	rVB2	160	113	0.01%	0.002%
48	8.475	2204	2219	2232	rVV3	8507	15343	1.62%	0.210%
49	8.549	2235	2242	2245	rBV	115	115	0.01%	0.002%
50	8.636	2255	2269	2295	rBV	267452	478290	50.35%	6.562%
51	8.790	2310	2317	2323	rBV5	2347	3489	0.37%	0.048%
52	9.160	2429	2432	2439	rVB2	255	282	0.03%	0.004%
53	9.417	2500	2512	2536	rBV	358026	591833	62.30%	8.120%
54	9.565	2555	2558	2562	rVV	232	235	0.02%	0.003%
55	9.603	2567	2570	2575	rVV	194	196	0.02%	0.003%
56	9.697	2590	2599	2606	rVB2	1278	1783	0.19%	0.024%
57	9.835	2639	2642	2650	rVB	128	131	0.01%	0.002%
58	10.099	2717	2724	2730	rBV2	428	643	0.07%	0.009%
59	10.128	2730	2733	2737	rVB2	256	191	0.02%	0.003%
60	10.671	2893	2902	2910	rVB3	2427	3576	0.38%	0.049%
61	10.758	2916	2929	2948	rVB	298418	477894	50.31%	6.556%
62	10.893	2956	2971	2983	rBV	11941	18950	1.99%	0.260%
63	11.121	3036	3042	3048	rVB2	618	678	0.07%	0.009%
64	11.160	3051	3054	3056	rVB	224	142	0.01%	0.002%
65	11.208	3064	3069	3073	rBV2	199	245	0.03%	0.003%
66	11.423	3133	3136	3138	rBV2	280	133	0.01%	0.002%
67	11.465	3140	3149	3160	rVB7	2706	5109	0.54%	0.070%
68	11.581	3180	3185	3187	rBV	176	184	0.02%	0.003%
69	11.697	3213	3221	3228	rVB3	1361	1903	0.20%	0.026%
70	11.812	3245	3257	3272	rBV	400239	632685	66.60%	8.680%
71	11.909	3284	3287	3289	rBV	140	128	0.01%	0.002%
72	11.938	3292	3296	3301	rVV5	803	987	0.10%	0.014%
73	11.973	3302	3307	3312	rVB2	1639	2111	0.22%	0.029%
74	12.063	3326	3335	3345	rBV3	5062	8553	0.90%	0.117%
75	12.099	3345	3346	3351	rVB2	350	230	0.02%	0.003%
76	12.195	3360	3376	3394	rVB	462770	751554	79.11%	10.311%

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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\SFAMULM112921WMA.M
 Title : VOC Analysis

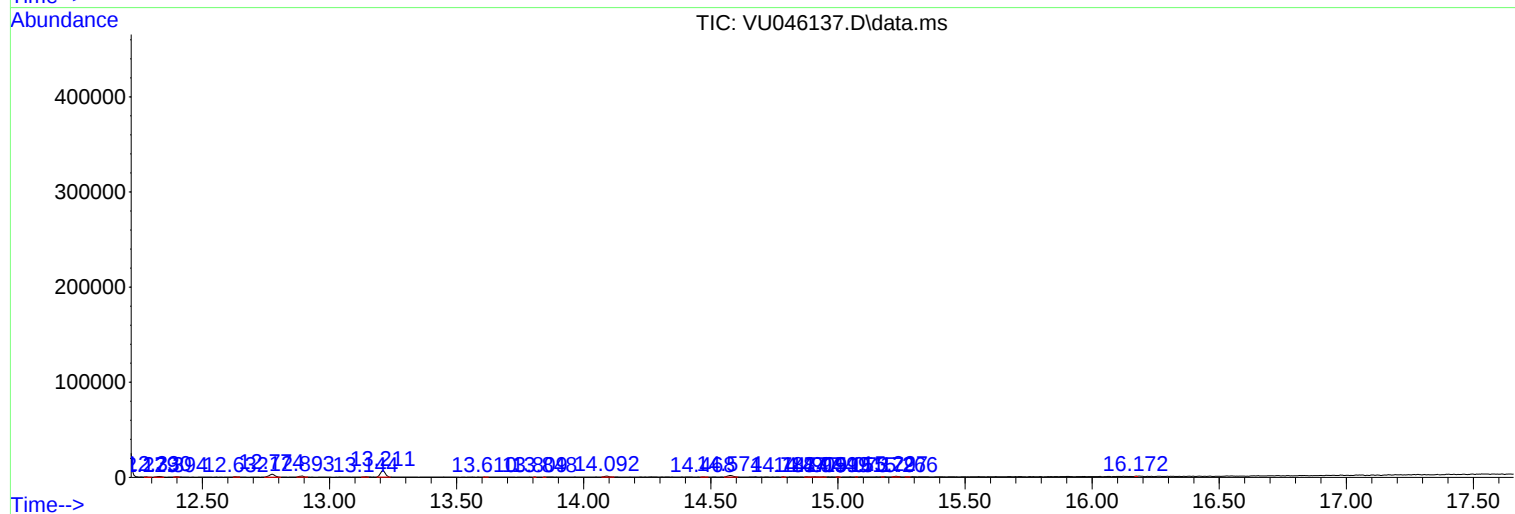
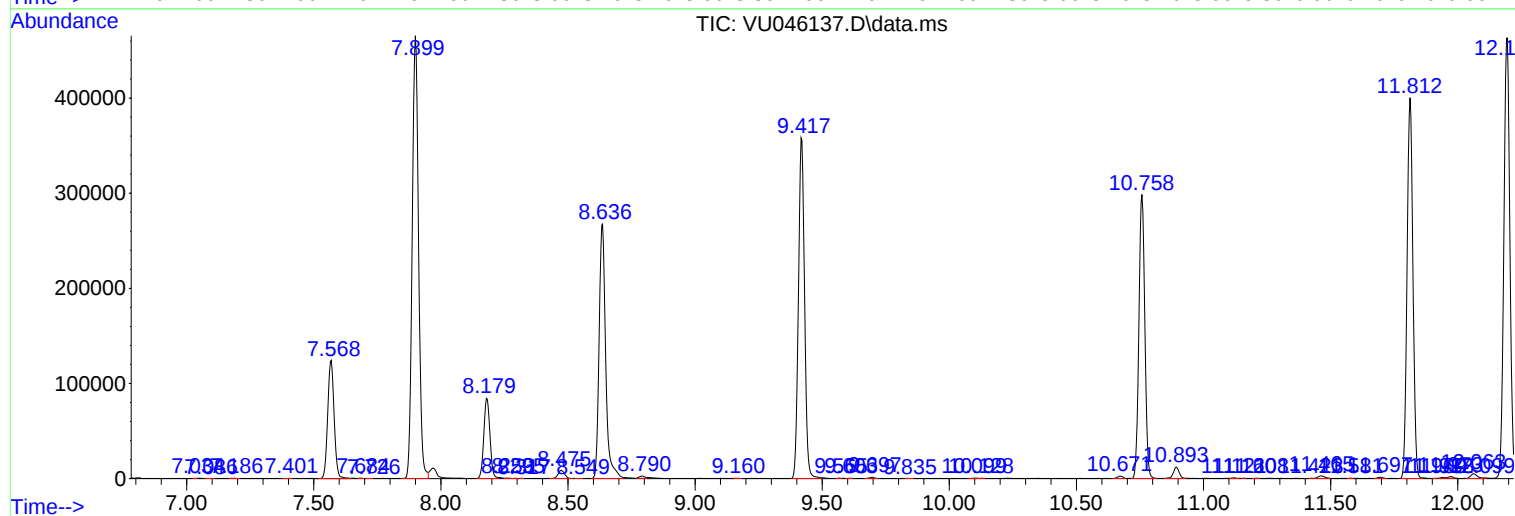
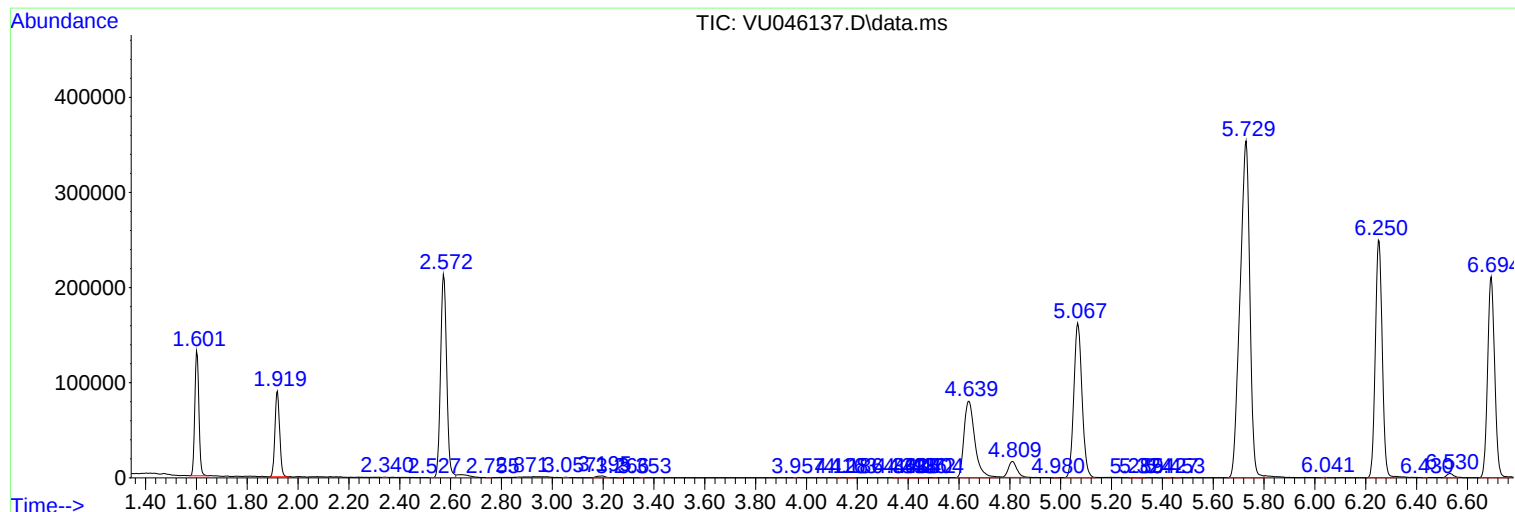
77	12.279	3400	3402	3409	rVB2	455	237	0.02%	0.003%
78	12.330	3411	3418	3424	rBV4	814	941	0.10%	0.013%
79	12.394	3435	3438	3443	rBV2	433	386	0.04%	0.005%
80	12.632	3508	3512	3517	rBV3	303	252	0.03%	0.003%
81	12.774	3547	3556	3567	rVB2	3196	4881	0.51%	0.067%
82	12.893	3586	3593	3600	rVB4	1171	1441	0.15%	0.020%
83	13.144	3665	3671	3674	rBV2	421	446	0.05%	0.006%
84	13.211	3684	3692	3701	rVB4	6679	9181	0.97%	0.126%
85	13.610	3814	3816	3821	rVB	197	112	0.01%	0.002%
86	13.809	3875	3878	3879	rBV	275	143	0.02%	0.002%
87	13.848	3887	3890	3891	rBV	227	111	0.01%	0.002%
88	14.092	3959	3966	3975	rBV2	1126	1540	0.16%	0.021%
89	14.468	4080	4083	4090	rBV	200	146	0.02%	0.002%
90	14.574	4109	4116	4126	rBV	1724	2657	0.28%	0.036%
91	14.787	4179	4182	4185	rVB	334	211	0.02%	0.003%
92	14.877	4207	4210	4215	rVB3	260	247	0.03%	0.003%
93	14.909	4215	4220	4226	rVB2	307	396	0.04%	0.005%
94	14.944	4226	4231	4234	rBV2	294	325	0.03%	0.004%
95	14.999	4246	4248	4252	rVB	420	235	0.02%	0.003%
96	15.073	4269	4271	4273	rBV	277	112	0.01%	0.002%
97	15.179	4301	4304	4305	rBV	268	137	0.01%	0.002%
98	15.227	4314	4319	4324	rBV3	629	591	0.06%	0.008%
99	15.266	4330	4331	4337	rBV2	218	210	0.02%	0.003%
100	16.172	4611	4613	4615	rBV	468	248	0.03%	0.003%

Sum of corrected areas: 7289014

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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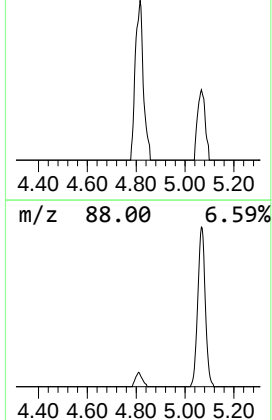
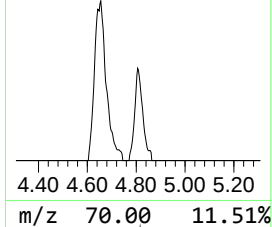
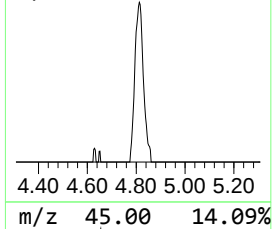
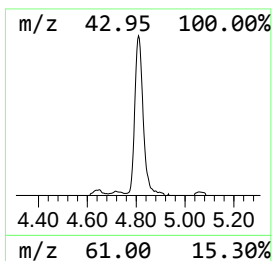
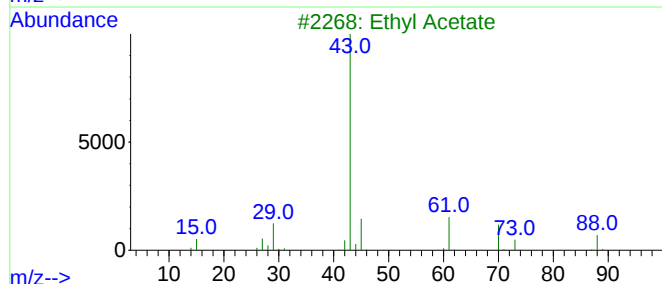
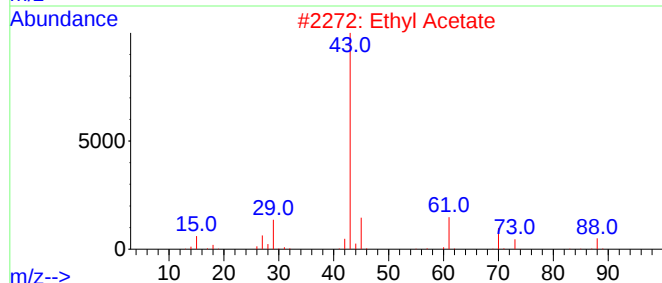
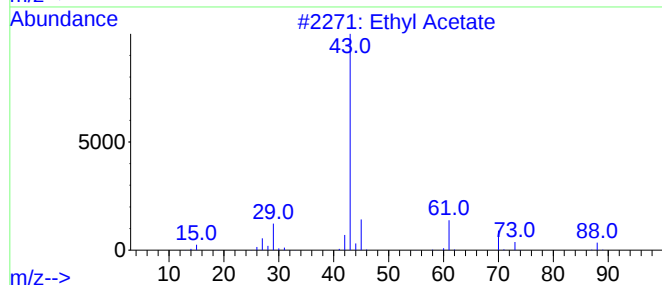
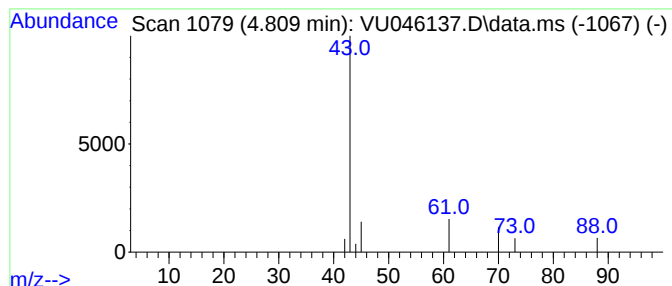
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.809	4.10 ug/L	38724	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	90
3			Ethyl Acetate	88	C4H8O2	000141-78-6	90
4			Ethyl Acetate	88	C4H8O2	000141-78-6	74
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	45



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl Acetate	4.809	4.1	ug/L	38724	1	6.253	472161	50.0