

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046136.D
 Acq On : 07 Dec 2021 13:33
 Operator : SY/MD
 Sample : M4960-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 10 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: VU046136.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	74	81	96	rVB	132278	146964	15.12%	2.014%
2	1.919	171	180	194	rVB	92991	119313	12.28%	1.635%
3	2.501	356	361	364	rBV2	381	393	0.04%	0.005%
4	2.572	371	383	400	rBV	220503	363202	37.38%	4.977%
5	2.800	452	454	459	rVB	336	250	0.03%	0.003%
6	3.192	563	576	587	rVB2	2897	6241	0.64%	0.086%
7	3.337	618	621	623	rBV	160	138	0.01%	0.002%
8	3.649	716	718	721	rVB	214	140	0.01%	0.002%
9	3.845	776	779	781	rBV	183	150	0.02%	0.002%
10	3.990	820	824	828	rVB2	205	167	0.02%	0.002%
11	4.247	899	904	907	rBB	149	179	0.02%	0.002%
12	4.276	907	913	917	rBV	167	274	0.03%	0.004%
13	4.314	922	925	928	rVV	268	230	0.02%	0.003%
14	4.456	966	969	971	rBV	150	128	0.01%	0.002%
15	4.488	977	979	981	rVB	290	139	0.01%	0.002%
16	4.639	1008	1026	1060	rBV	80729	249679	25.69%	3.421%
17	4.809	1068	1079	1106	rVB3	16266	39114	4.03%	0.536%
18	5.067	1142	1159	1182	rBV	167439	374827	38.57%	5.136%
19	5.157	1182	1187	1191	rBV2	207	270	0.03%	0.004%
20	5.182	1191	1195	1197	rBV2	258	242	0.02%	0.003%
21	5.285	1225	1227	1231	rVB	267	169	0.02%	0.002%
22	5.414	1263	1267	1269	rBV	245	206	0.02%	0.003%
23	5.449	1274	1278	1279	rBV	143	123	0.01%	0.002%
24	5.594	1320	1323	1327	rVB	174	168	0.02%	0.002%
25	5.729	1343	1365	1384	rBV2	364084	971746	100.00%	13.315%
26	6.009	1449	1452	1455	rVB	201	150	0.02%	0.002%
27	6.044	1459	1463	1468	rBV2	401	444	0.05%	0.006%
28	6.070	1468	1471	1474	rVB	237	172	0.02%	0.002%
29	6.192	1504	1509	1510	rBV	169	168	0.02%	0.002%
30	6.250	1512	1527	1546	rBV	227681	429014	44.15%	5.878%
31	6.530	1606	1614	1630	rVB7	3557	7806	0.80%	0.107%
32	6.694	1650	1665	1682	rBV	215135	417055	42.92%	5.714%
33	6.796	1694	1697	1700	rBV2	410	310	0.03%	0.004%
34	6.832	1706	1708	1713	rVB2	369	172	0.02%	0.002%
35	7.041	1769	1773	1781	rVB2	578	720	0.07%	0.010%
36	7.089	1786	1788	1791	rBV	278	188	0.02%	0.003%

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Integrator: RTE

Smoothing : OFF

Filtering: 5

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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_U\Method\SFAMULM112921WMA.M

Title : VOC Analysis

37	7.186	1811	1818	1824	rVB2	419	696	0.07%	0.010%
38	7.214	1824	1827	1829	rBV	161	129	0.01%	0.002%
39	7.501	1912	1916	1919	rBV	161	189	0.02%	0.003%
40	7.568	1923	1937	1950	rBV	124454	218405	22.48%	2.993%
41	7.800	2005	2009	2011	rBV	283	211	0.02%	0.003%
42	7.838	2017	2021	2025	rVB2	199	147	0.02%	0.002%
43	7.899	2025	2040	2055	rBV	468549	816732	84.05%	11.191%
44	8.121	2104	2109	2115	rBV	101	120	0.01%	0.002%
45	8.179	2115	2127	2153	rBV	86660	146256	15.05%	2.004%
46	8.333	2172	2175	2180	rVB	219	166	0.02%	0.002%
47	8.472	2206	2218	2232	rBV2	9137	16282	1.68%	0.223%
48	8.568	2246	2248	2252	rVB2	250	143	0.01%	0.002%
49	8.636	2256	2269	2308	rBV	279721	501046	51.56%	6.865%
50	8.793	2309	2318	2324	rBV5	3170	4885	0.50%	0.067%
51	9.163	2429	2433	2437	rVB2	308	258	0.03%	0.004%
52	9.321	2479	2482	2489	rBV	195	166	0.02%	0.002%
53	9.417	2499	2512	2549	rVB	322755	541908	55.77%	7.425%
54	9.568	2552	2559	2565	rBV2	489	594	0.06%	0.008%
55	9.693	2592	2598	2608	rVB3	1394	1810	0.19%	0.025%
56	10.108	2720	2727	2731	rBV2	557	680	0.07%	0.009%
57	10.230	2762	2765	2766	rBV	231	126	0.01%	0.002%
58	10.292	2781	2784	2788	rBV2	183	142	0.01%	0.002%
59	10.340	2794	2799	2806	rBV	144	214	0.02%	0.003%
60	10.420	2822	2824	2829	rVB	236	151	0.02%	0.002%
61	10.674	2895	2903	2912	rVB	3010	3916	0.40%	0.054%
62	10.758	2916	2929	2947	rVB	311502	496266	51.07%	6.800%
63	10.893	2957	2971	2988	rBV3	11266	17981	1.85%	0.246%
64	10.999	3001	3004	3006	rBV	174	132	0.01%	0.002%
65	11.092	3028	3033	3035	rBV	256	225	0.02%	0.003%
66	11.108	3035	3038	3039	rVV2	257	163	0.02%	0.002%
67	11.118	3039	3041	3048	rVB2	709	597	0.06%	0.008%
68	11.150	3048	3051	3053	rBV2	280	161	0.02%	0.002%
69	11.205	3066	3068	3071	rVB	217	121	0.01%	0.002%
70	11.295	3092	3096	3101	rBB2	176	167	0.02%	0.002%
71	11.385	3120	3124	3127	rBV	330	213	0.02%	0.003%
72	11.459	3138	3147	3159	rBV5	2767	5555	0.57%	0.076%
73	11.568	3177	3181	3182	rBV	264	159	0.02%	0.002%
74	11.578	3182	3184	3192	rVB2	371	443	0.05%	0.006%
75	11.693	3213	3220	3226	rVB4	1827	2271	0.23%	0.031%
76	11.812	3245	3257	3272	rBV	374974	581580	59.85%	7.969%

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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

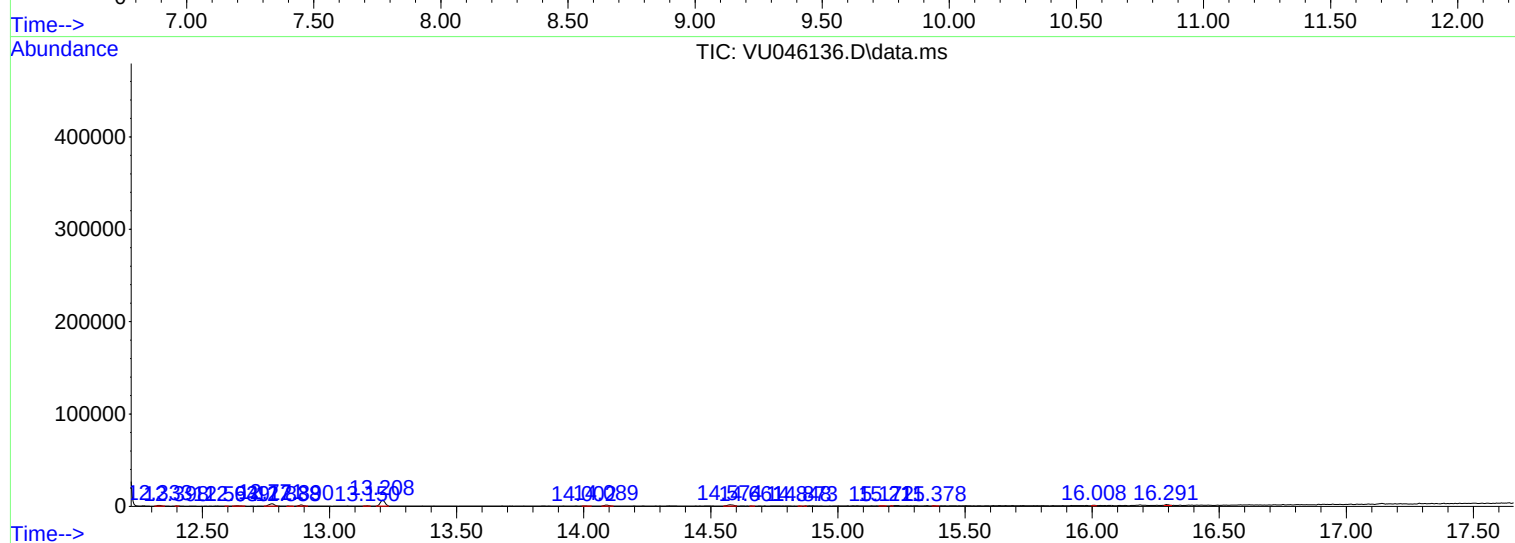
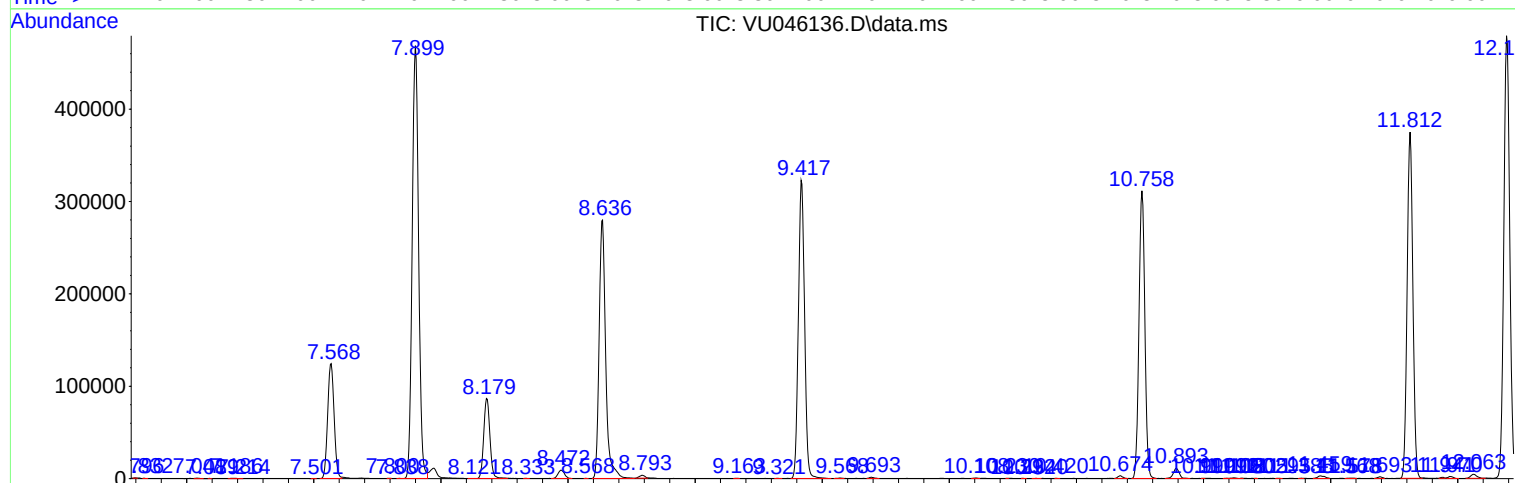
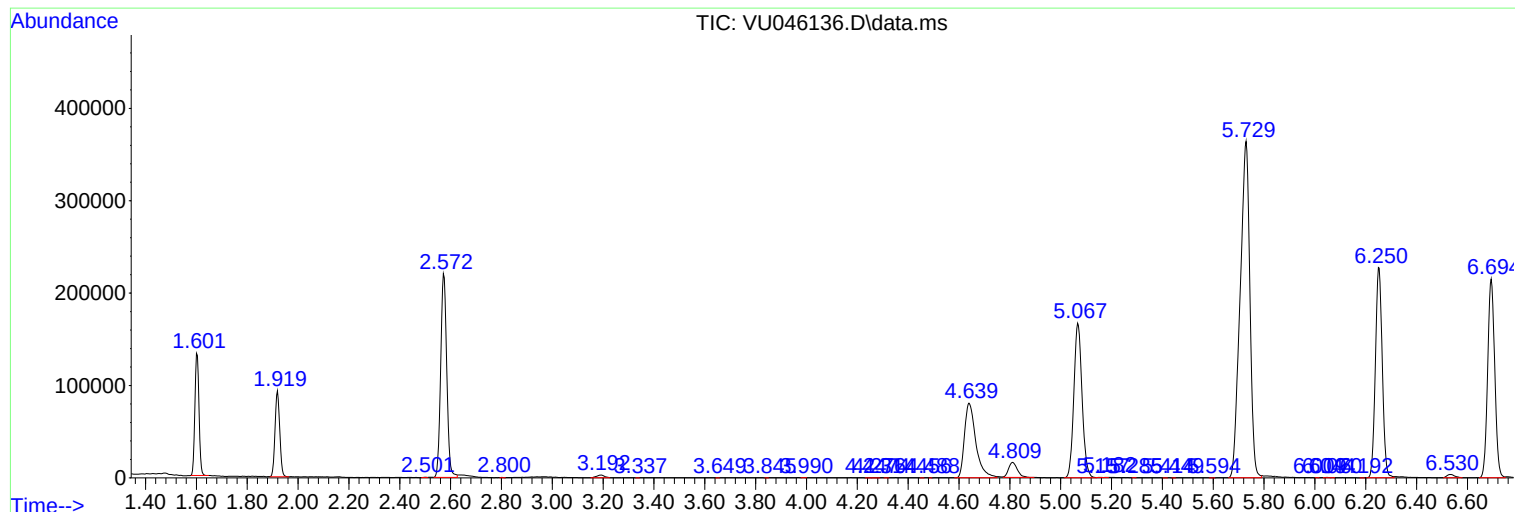
77	11.941	3292	3297	3300	rVV4	1137	1148	0.12%	0.016%
78	11.970	3302	3306	3317	rVB3	2153	2906	0.30%	0.040%
79	12.063	3325	3335	3349	rBV2	4430	7951	0.82%	0.109%
80	12.192	3359	3375	3391	rBV	479032	770781	79.32%	10.561%
81	12.333	3412	3419	3425	rVB4	810	992	0.10%	0.014%
82	12.398	3437	3439	3442	rBV	290	159	0.02%	0.002%
83	12.594	3498	3500	3503	rBV2	163	128	0.01%	0.002%
84	12.639	3507	3514	3523	rBV3	454	662	0.07%	0.009%
85	12.771	3546	3555	3563	rBV2	2538	4005	0.41%	0.055%
86	12.838	3574	3576	3583	rVB2	337	213	0.02%	0.003%
87	12.890	3586	3592	3600	rVB4	1258	1493	0.15%	0.020%
88	13.150	3667	3673	3677	rVB3	387	433	0.04%	0.006%
89	13.208	3683	3691	3699	rVV3	6388	8516	0.88%	0.117%
90	14.002	3935	3938	3947	rVB	271	314	0.03%	0.004%
91	14.089	3959	3965	3974	rVB2	1118	1504	0.15%	0.021%
92	14.574	4108	4116	4125	rBV3	1408	2438	0.25%	0.033%
93	14.661	4140	4143	4147	rBV2	183	142	0.01%	0.002%
94	14.848	4199	4201	4205	rBV	226	124	0.01%	0.002%
95	14.873	4206	4209	4210	rBV2	257	157	0.02%	0.002%
96	15.172	4298	4302	4308	rBV2	304	347	0.04%	0.005%
97	15.211	4312	4314	4316	rBV2	245	141	0.01%	0.002%
98	15.378	4363	4366	4372	rVB	346	229	0.02%	0.003%
99	16.008	4558	4562	4565	rBV	507	470	0.05%	0.006%
100	16.291	4647	4650	4657	rBV5	953	905	0.09%	0.012%

Sum of corrected areas: 7298215

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ALS Vial : 10 Sample Multiplier: 1

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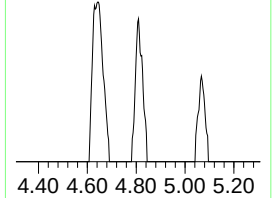
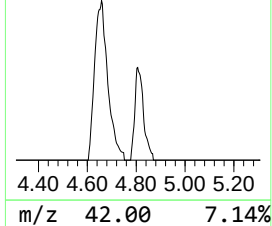
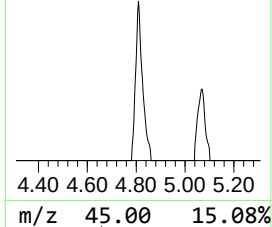
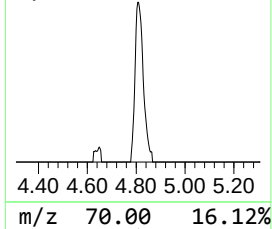
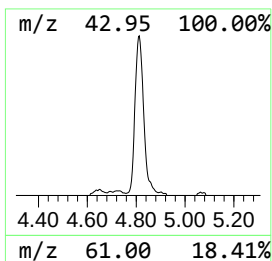
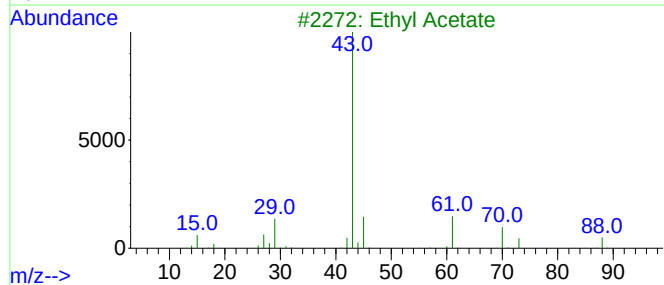
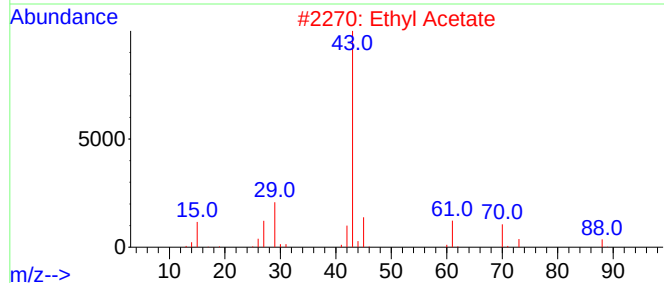
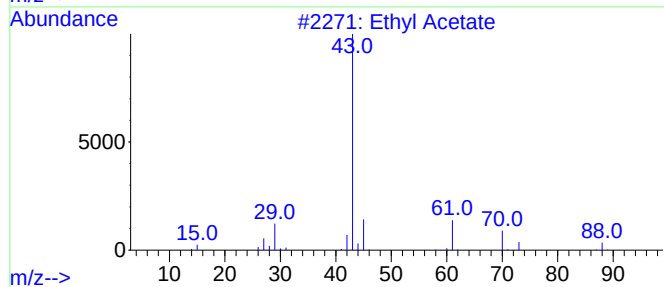
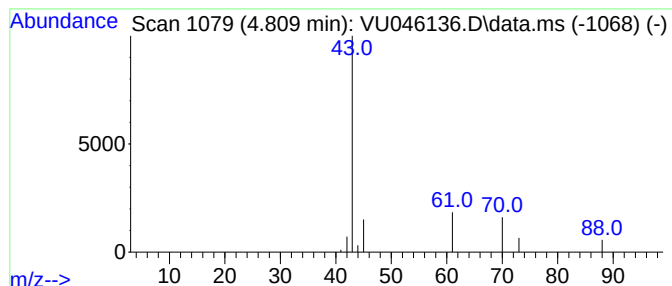
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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	4.56 ug/L	39114	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	83
2			Ethyl Acetate	88	C4H8O2	000141-78-6	83
3			Ethyl Acetate	88	C4H8O2	000141-78-6	83
4			Ethyl Acetate	88	C4H8O2	000141-78-6	83
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	74



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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	4.6	ug/L	39114	1	6.253	429014	50.0