

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071422\
 Data File : VU049720.D
 Acq On : 14 Jul 2022 15:27
 Operator : SY/MD
 Sample : N3722-18
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5D24

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\SFAMULM071122WMA.M
 Title : VOC Analysis

Signal : TIC: VU049720.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	39	44	50	rBV3	2823	3211	0.42%	0.049%
2	1.517	50	55	65	rVV3	2853	4135	0.54%	0.064%
3	1.594	70	79	96	rVB	88095	105981	13.82%	1.629%
4	1.681	99	106	119	rBV	26304	31049	4.05%	0.477%
5	1.899	166	174	191	rVB	67384	87454	11.41%	1.344%
6	2.243	276	281	285	rBV4	540	643	0.08%	0.010%
7	2.295	286	297	304	rVV2	3900	6872	0.90%	0.106%
8	2.375	315	322	332	rVB5	2028	3283	0.43%	0.050%
9	2.562	367	380	392	rBV	131179	211674	27.61%	3.253%
10	2.629	393	401	421	rVB3	9784	17873	2.33%	0.275%
11	2.764	436	443	444	rBV3	816	899	0.12%	0.014%
12	2.887	478	481	482	rBV2	407	261	0.03%	0.004%
13	2.899	483	485	491	rVB2	535	513	0.07%	0.008%
14	2.938	491	497	499	rBV	384	402	0.05%	0.006%
15	3.038	525	528	531	rBV	526	414	0.05%	0.006%
16	3.182	562	573	590	rVB4	4657	10642	1.39%	0.164%
17	3.272	598	601	604	rBV2	263	273	0.04%	0.004%
18	3.485	663	667	671	rBV	189	181	0.02%	0.003%
19	3.517	674	677	681	rVB	249	192	0.03%	0.003%
20	3.678	721	727	729	rBV	211	226	0.03%	0.003%
21	3.809	764	768	772	rBV2	226	211	0.03%	0.003%
22	3.845	776	779	782	rBV	268	223	0.03%	0.003%
23	3.880	788	790	795	rVB	309	245	0.03%	0.004%
24	3.948	805	811	814	rBV2	216	196	0.03%	0.003%
25	4.012	827	831	834	rBV2	148	174	0.02%	0.003%
26	4.231	896	899	907	rBV2	243	275	0.04%	0.004%
27	4.440	955	964	969	rBV4	1557	3026	0.39%	0.047%
28	4.485	977	978	983	rVB2	374	219	0.03%	0.003%
29	4.620	1008	1020	1046	rBV	103345	250708	32.70%	3.853%
30	4.800	1063	1076	1106	rBV	260392	557632	72.74%	8.569%
31	5.060	1142	1157	1178	rBV	139399	303631	39.61%	4.666%
32	5.198	1195	1200	1202	rBV3	316	293	0.04%	0.005%
33	5.288	1222	1228	1236	rBV3	831	1173	0.15%	0.018%
34	5.353	1245	1248	1250	rBV	269	207	0.03%	0.003%
35	5.372	1250	1254	1255	rBV2	453	353	0.05%	0.005%
36	5.423	1267	1270	1275	rBV2	175	196	0.03%	0.003%

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37	5.536	1300	1305	1306	rBV	254	177	0.02%	0.003%
38	5.603	1321	1326	1329	rBV	339	364	0.05%	0.006%
39	5.722	1342	1363	1386	rBV2	281260	766622	100.00%	11.781%
40	5.973	1435	1441	1444	rBV3	320	354	0.05%	0.005%
41	6.073	1469	1472	1478	rVV2	227	218	0.03%	0.003%
42	6.185	1502	1507	1512	rBV2	301	349	0.05%	0.005%
43	6.247	1512	1526	1548	rBV	243626	461739	60.23%	7.096%
44	6.430	1579	1583	1587	rBV3	371	360	0.05%	0.006%
45	6.523	1606	1612	1619	rVV3	1621	2369	0.31%	0.036%
46	6.629	1643	1645	1648	rVB	342	175	0.02%	0.003%
47	6.690	1648	1664	1685	rBV	191129	366448	47.80%	5.631%
48	6.771	1685	1689	1691	rBV2	274	174	0.02%	0.003%
49	6.886	1717	1725	1728	rBV2	611	651	0.08%	0.010%
50	6.983	1750	1755	1760	rVB2	328	323	0.04%	0.005%
51	7.124	1794	1799	1802	rVV4	325	292	0.04%	0.004%
52	7.189	1806	1819	1825	rBV6	789	1616	0.21%	0.025%
53	7.272	1842	1845	1847	rBV	216	171	0.02%	0.003%
54	7.292	1847	1851	1854	rVV2	158	171	0.02%	0.003%
55	7.417	1883	1890	1892	rBV2	219	209	0.03%	0.003%
56	7.488	1907	1912	1915	rBV2	175	192	0.03%	0.003%
57	7.565	1923	1936	1954	rVV	92072	159463	20.80%	2.450%
58	7.793	2002	2007	2012	rVB2	542	573	0.07%	0.009%
59	7.828	2015	2018	2024	rVB	197	169	0.02%	0.003%
60	7.896	2025	2039	2057	rBV	315838	534794	69.76%	8.218%
61	8.179	2115	2127	2143	rBV	61277	104039	13.57%	1.599%
62	8.436	2202	2207	2212	rBV2	539	627	0.08%	0.010%
63	8.632	2256	2268	2299	rBV2	282639	528734	68.97%	8.125%
64	8.787	2309	2316	2326	rVB8	4339	6687	0.87%	0.103%
65	8.957	2365	2369	2372	rBV	281	184	0.02%	0.003%
66	9.417	2498	2512	2534	rBV	336970	560976	73.18%	8.621%
67	9.713	2601	2604	2608	rBV2	228	217	0.03%	0.003%
68	9.758	2614	2618	2621	rBV2	246	212	0.03%	0.003%
69	10.240	2761	2768	2776	rBV4	1578	2650	0.35%	0.041%
70	10.352	2798	2803	2811	rVB6	843	1065	0.14%	0.016%
71	10.426	2823	2826	2829	rBV2	246	190	0.02%	0.003%
72	10.491	2840	2846	2849	rBV2	191	213	0.03%	0.003%
73	10.590	2873	2877	2883	rBV	267	328	0.04%	0.005%
74	10.664	2897	2900	2904	rBV	192	217	0.03%	0.003%
75	10.754	2916	2928	2946	rBV	261045	420576	54.86%	6.463%
76	10.877	2963	2966	2968	rVB2	360	234	0.03%	0.004%

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 Title : VOC Analysis

77	10.999	3001	3004	3008	rBV	239	222	0.03%	0.003%
78	11.115	3038	3040	3045	rVB	333	246	0.03%	0.004%
79	11.301	3094	3098	3099	rBV2	246	178	0.02%	0.003%
80	11.340	3107	3110	3115	rBV2	233	183	0.02%	0.003%
81	11.423	3133	3136	3142	rVB	340	295	0.04%	0.005%
82	11.481	3149	3154	3158	rBV3	918	867	0.11%	0.013%
83	11.696	3217	3221	3225	rVB3	261	238	0.03%	0.004%
84	11.812	3245	3257	3280	rBV	305299	484770	63.23%	7.450%
85	12.005	3315	3317	3321	rBV2	309	189	0.02%	0.003%
86	12.066	3327	3336	3354	rBV4	8136	15533	2.03%	0.239%
87	12.192	3363	3375	3394	rBV	290580	468550	61.12%	7.200%
88	12.352	3422	3425	3428	rBV2	309	203	0.03%	0.003%
89	12.397	3436	3439	3442	rBV2	312	229	0.03%	0.004%
90	12.870	3583	3586	3589	rBV2	303	209	0.03%	0.003%
91	12.896	3589	3594	3599	rVB3	1051	945	0.12%	0.015%
92	12.960	3612	3614	3621	rVB2	335	301	0.04%	0.005%
93	13.214	3687	3693	3703	rVB5	1420	1998	0.26%	0.031%
94	13.256	3703	3706	3710	rBV	328	303	0.04%	0.005%
95	13.992	3932	3935	3937	rBV2	355	212	0.03%	0.003%
96	14.008	3937	3940	3943	rVV	383	273	0.04%	0.004%
97	14.217	4001	4005	4009	rBV3	322	283	0.04%	0.004%
98	14.240	4009	4012	4016	rBV3	365	326	0.04%	0.005%
99	14.870	4205	4208	4212	rBV2	481	399	0.05%	0.006%
100	15.404	4372	4374	4378	rBV2	384	356	0.05%	0.005%

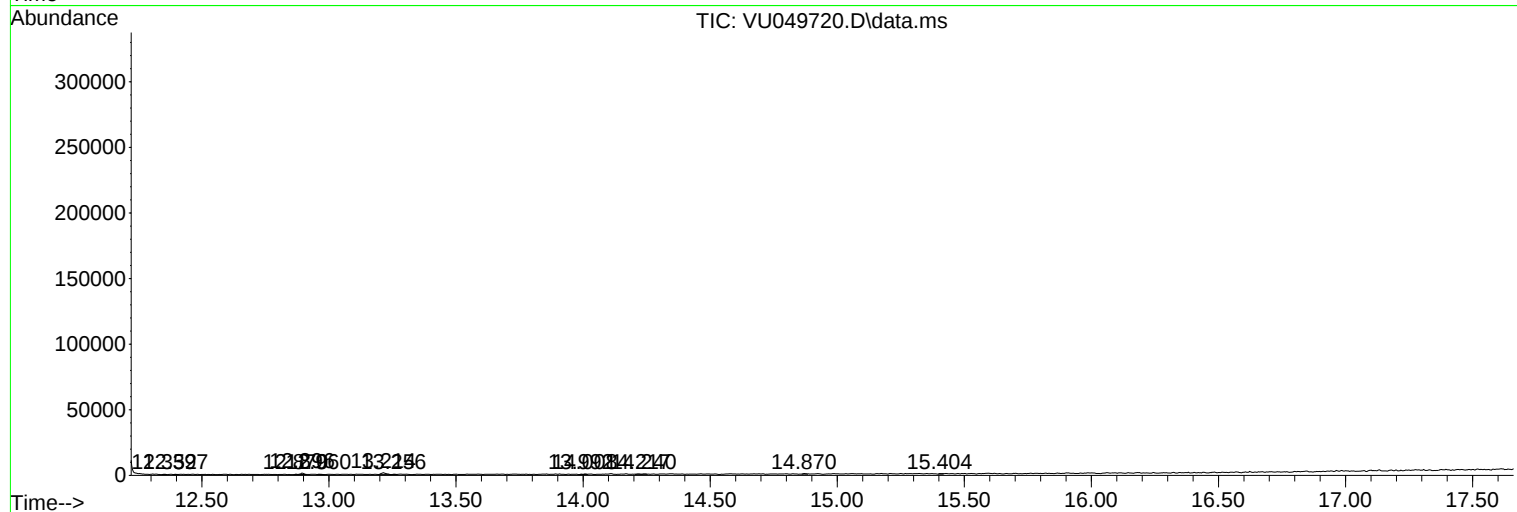
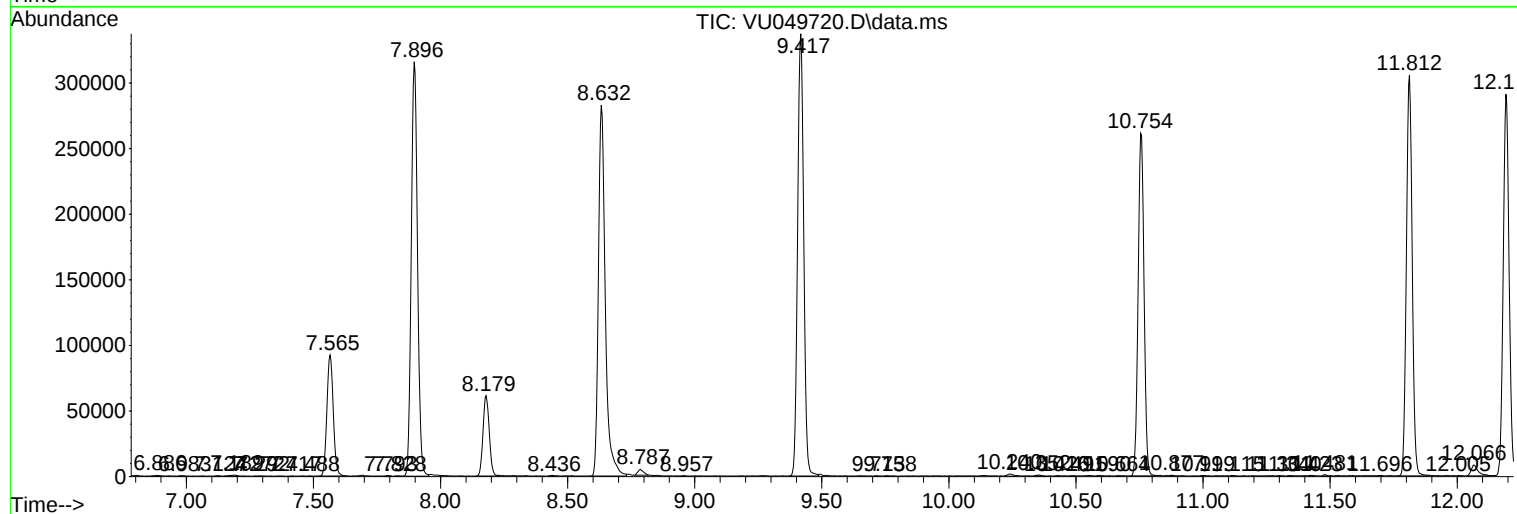
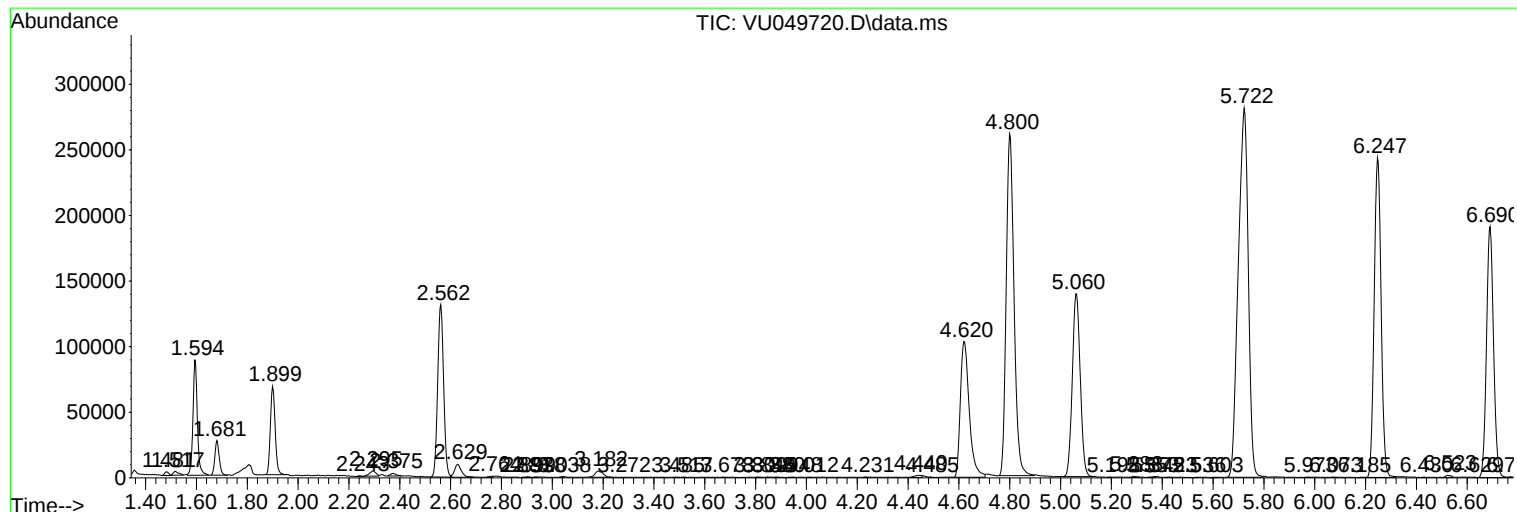
Sum of corrected areas: 6507370

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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



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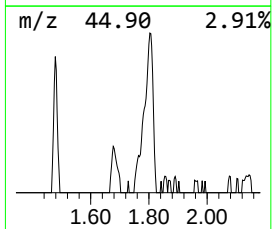
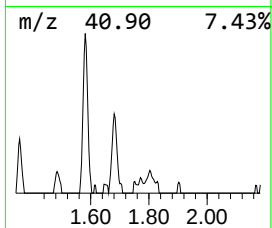
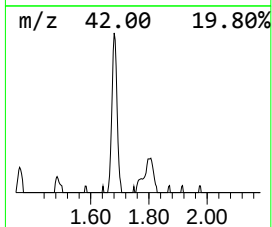
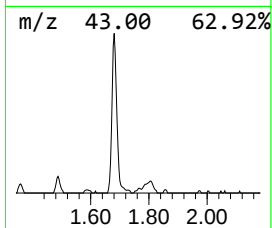
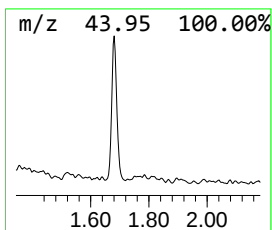
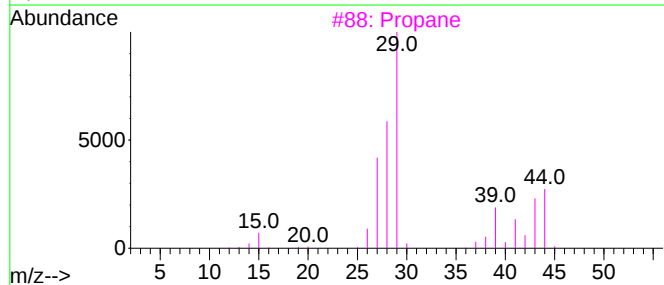
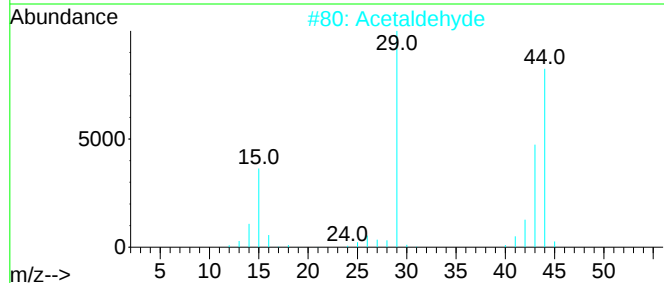
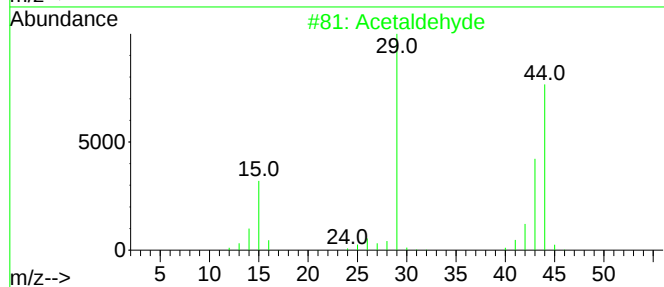
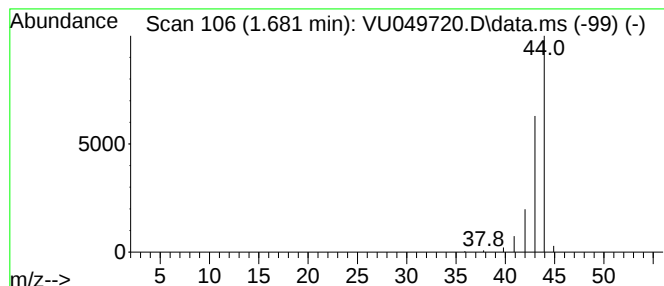
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.681	3.36 ug/L	31049	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Acetaldehyde	44	C2H4O	000075-07-0	74
3			Propane	44	C3H8	000074-98-6	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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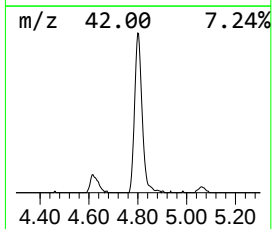
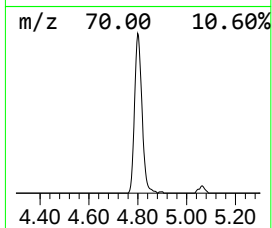
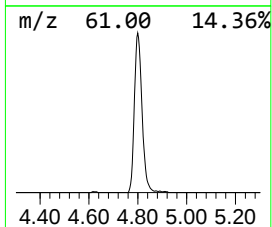
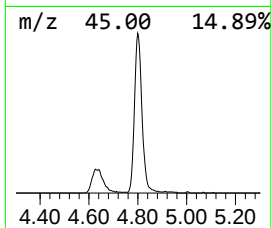
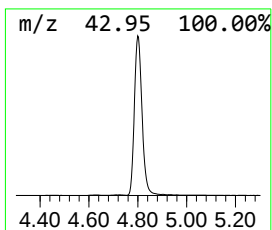
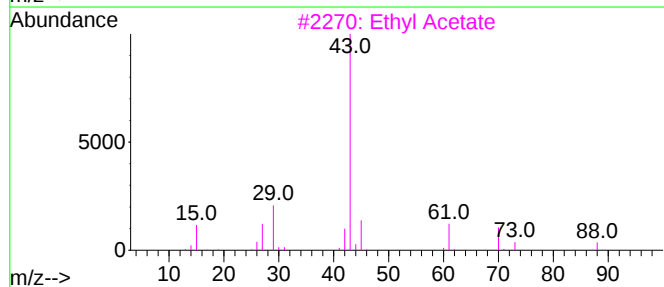
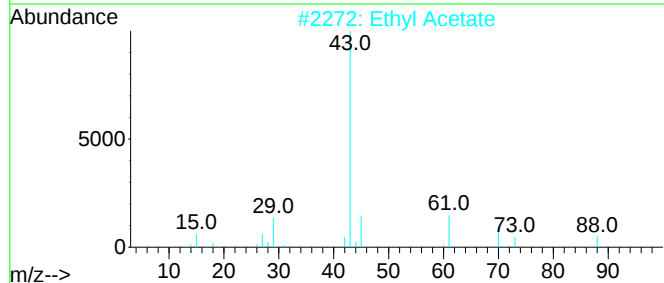
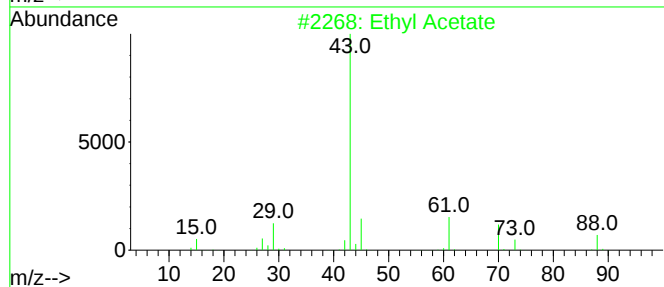
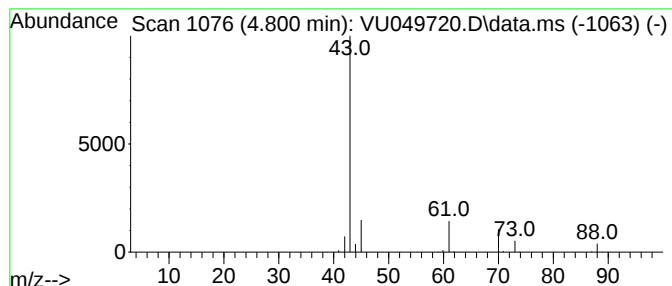
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.800	60.38 ug/L	557632	1,4-Difluorobenzene	6.247

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	86
4			Ethyl Acetate	88	C4H8O2	000141-78-6	86
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.681	3.4	ug/L	31049	1	6.247	461739	50.0
Ethyl Acetate	4.800	60.4	ug/L	557632	1	6.247	461739	50.0