

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120221\
 Data File : VU046058.D
 Acq On : 02 Dec 2021 17:27
 Operator : SY/MD
 Sample : PB141128TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB128

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: VU046058.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	73	81	95	rBV	102842	113047	12.74%	1.432%
2	1.916	170	179	192	rBV	77704	98436	11.09%	1.247%
3	2.382	316	324	330	rBV4	1650	2545	0.29%	0.032%
4	2.572	370	383	401	rBV	179576	299552	33.75%	3.795%
5	2.835	462	465	471	rBV2	183	241	0.03%	0.003%
6	2.954	496	502	509	rBV	327	447	0.05%	0.006%
7	3.051	523	532	544	rBV4	2916	5231	0.59%	0.066%
8	3.182	565	573	587	rBV	1703	3716	0.42%	0.047%
9	3.832	767	775	778	rBV3	1027	1370	0.15%	0.017%
10	4.137	865	870	876	rBB	150	237	0.03%	0.003%
11	4.324	922	928	932	rBB	171	248	0.03%	0.003%
12	4.369	937	942	947	rBV	177	270	0.03%	0.003%
13	4.469	970	973	979	rBV	156	243	0.03%	0.003%
14	4.629	1008	1023	1060	rVV	93420	245211	27.63%	3.106%
15	4.954	1122	1124	1129	rBV	289	248	0.03%	0.003%
16	5.067	1143	1159	1180	rBV	155345	344009	38.76%	4.358%
17	5.729	1343	1365	1387	rBV2	329248	887521	100.00%	11.243%
18	5.877	1408	1411	1414	rBV	249	222	0.03%	0.003%
19	5.909	1418	1421	1423	rBV2	736	474	0.05%	0.006%
20	6.250	1513	1527	1545	rBV	303464	572752	64.53%	7.256%
21	6.533	1604	1615	1636	rBV2	6767	13497	1.52%	0.171%
22	6.694	1650	1665	1681	rBV	206000	397767	44.82%	5.039%
23	6.890	1722	1726	1729	rBV	316	263	0.03%	0.003%
24	6.925	1729	1737	1751	rVV3	1094	2377	0.27%	0.030%
25	7.041	1760	1773	1793	rBV	86701	152627	17.20%	1.934%
26	7.182	1810	1817	1827	rVB4	2916	4601	0.52%	0.058%
27	7.485	1907	1911	1914	rBV	318	234	0.03%	0.003%
28	7.568	1923	1937	1955	rBV	118063	201105	22.66%	2.548%
29	7.687	1966	1974	1981	rBV3	1664	2100	0.24%	0.027%
30	7.739	1981	1990	2002	rVB	12066	19258	2.17%	0.244%
31	7.899	2026	2040	2057	rBV	419528	728158	82.04%	9.225%
32	8.089	2095	2099	2105	rVB3	442	445	0.05%	0.006%
33	8.182	2114	2128	2148	rBV	80830	134622	15.17%	1.705%
34	8.462	2208	2215	2224	rVB2	2740	4053	0.46%	0.051%
35	8.574	2238	2250	2257	rBV3	8744	13613	1.53%	0.172%
36	8.632	2257	2268	2288	rVV	271873	486827	54.85%	6.167%

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

37	8.729	2289	2298	2313	rVB	140344	220087	24.80%	2.788%
38	8.835	2321	2331	2343	rVB2	14432	22380	2.52%	0.284%
39	8.915	2349	2356	2359	rBV3	455	666	0.08%	0.008%
40	9.211	2437	2448	2461	rBV	70920	109261	12.31%	1.384%
41	9.343	2484	2489	2490	rBV	303	257	0.03%	0.003%
42	9.420	2500	2513	2549	rVB	428193	725292	81.72%	9.188%
43	9.574	2554	2561	2571	rBV	1473	2144	0.24%	0.027%
44	9.693	2588	2598	2608	rBV3	6353	10068	1.13%	0.128%
45	9.745	2608	2614	2621	rVB3	2346	2924	0.33%	0.037%
46	10.073	2709	2716	2723	rBV3	2303	3512	0.40%	0.044%
47	10.111	2726	2728	2738	rVV4	1053	1143	0.13%	0.014%
48	10.253	2764	2772	2779	rBV3	2164	2939	0.33%	0.037%
49	10.353	2796	2803	2810	rVB4	627	757	0.09%	0.010%
50	10.398	2811	2817	2823	rVB3	974	1148	0.13%	0.015%
51	10.558	2860	2867	2876	rVV3	1350	1927	0.22%	0.024%
52	10.600	2876	2880	2881	rVV2	825	611	0.07%	0.008%
53	10.626	2882	2888	2892	rVV3	2691	3630	0.41%	0.046%
54	10.664	2892	2900	2911	rVB5	3542	7615	0.86%	0.096%
55	10.758	2916	2929	2945	rBV	294307	467462	52.67%	5.922%
56	10.867	2960	2963	2968	rBV2	543	510	0.06%	0.006%
57	10.957	2986	2991	2994	rBV2	342	289	0.03%	0.004%
58	11.002	2998	3005	3011	rBV4	880	1460	0.16%	0.018%
59	11.066	3018	3025	3027	rBV3	945	1168	0.13%	0.015%
60	11.115	3032	3040	3057	rVB2	9740	15860	1.79%	0.201%
61	11.205	3064	3068	3072	rBV3	530	372	0.04%	0.005%
62	11.291	3088	3095	3097	rBV3	592	626	0.07%	0.008%
63	11.314	3097	3102	3110	rVB4	1429	1892	0.21%	0.024%
64	11.378	3112	3122	3127	rBV5	1713	2917	0.33%	0.037%
65	11.417	3128	3134	3140	rVV3	5609	7188	0.81%	0.091%
66	11.465	3143	3149	3156	rVB5	3365	5364	0.60%	0.068%
67	11.574	3176	3183	3190	rBV3	2470	3501	0.39%	0.044%
68	11.639	3199	3203	3212	rVB4	1550	2393	0.27%	0.030%
69	11.706	3212	3224	3233	rBV6	4907	10023	1.13%	0.127%
70	11.748	3235	3237	3243	rVB3	701	539	0.06%	0.007%
71	11.812	3245	3257	3271	rBV	478292	759948	85.63%	9.627%
72	11.912	3284	3288	3293	rBV2	2785	2663	0.30%	0.034%
73	12.118	3349	3352	3356	rBV3	730	699	0.08%	0.009%
74	12.195	3360	3376	3391	rVB	433804	699489	78.81%	8.861%
75	12.256	3392	3395	3396	rBV	414	231	0.03%	0.003%
76	12.327	3409	3417	3427	rBV3	11167	16128	1.82%	0.204%

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 Title : VOC Analysis

77	12.388	3427	3436	3437	rBV4	1321	1401	0.16%	0.018%
78	12.484	3464	3466	3468	rBV2	630	385	0.04%	0.005%
79	12.603	3498	3503	3509	rBV4	595	703	0.08%	0.009%
80	12.635	3509	3513	3517	rVV2	815	857	0.10%	0.011%
81	12.668	3517	3523	3530	rVB5	1432	2025	0.23%	0.026%
82	12.838	3565	3576	3579	rVB5	697	948	0.11%	0.012%
83	12.928	3597	3604	3613	rBV4	1317	2519	0.28%	0.032%
84	13.005	3624	3628	3633	rVB	814	724	0.08%	0.009%
85	13.047	3633	3641	3647	rVB5	1111	1600	0.18%	0.020%
86	13.137	3661	3669	3673	rBV4	1137	1396	0.16%	0.018%
87	13.433	3755	3761	3767	rVB2	1903	2318	0.26%	0.029%
88	13.581	3804	3807	3812	rBV3	755	804	0.09%	0.010%
89	14.089	3955	3965	3973	rBV2	4700	6674	0.75%	0.085%
90	14.192	3995	3997	4010	rVB3	723	789	0.09%	0.010%
91	14.452	4072	4078	4082	rVB2	1060	1095	0.12%	0.014%
92	14.571	4112	4115	4119	rBV2	469	443	0.05%	0.006%
93	14.873	4206	4209	4214	rVB2	357	284	0.03%	0.004%
94	15.050	4259	4264	4267	rBV2	248	260	0.03%	0.003%
95	15.227	4311	4319	4327	rBV3	4732	7326	0.83%	0.093%
96	15.346	4350	4356	4360	rBV2	350	465	0.05%	0.006%
97	15.407	4369	4375	4384	rBV7	2296	3946	0.44%	0.050%
98	15.954	4541	4545	4554	rBV3	970	1219	0.14%	0.015%
99	16.208	4621	4624	4628	rVB3	573	371	0.04%	0.005%
100	16.516	4718	4720	4726	rVB3	662	495	0.06%	0.006%

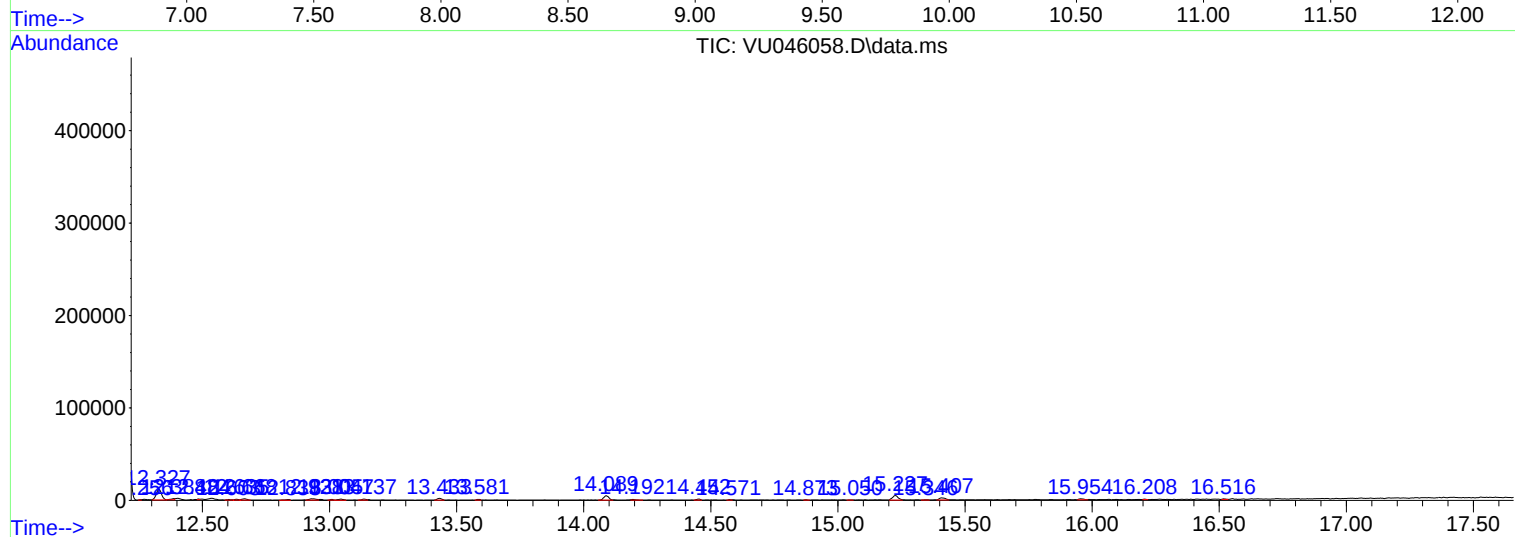
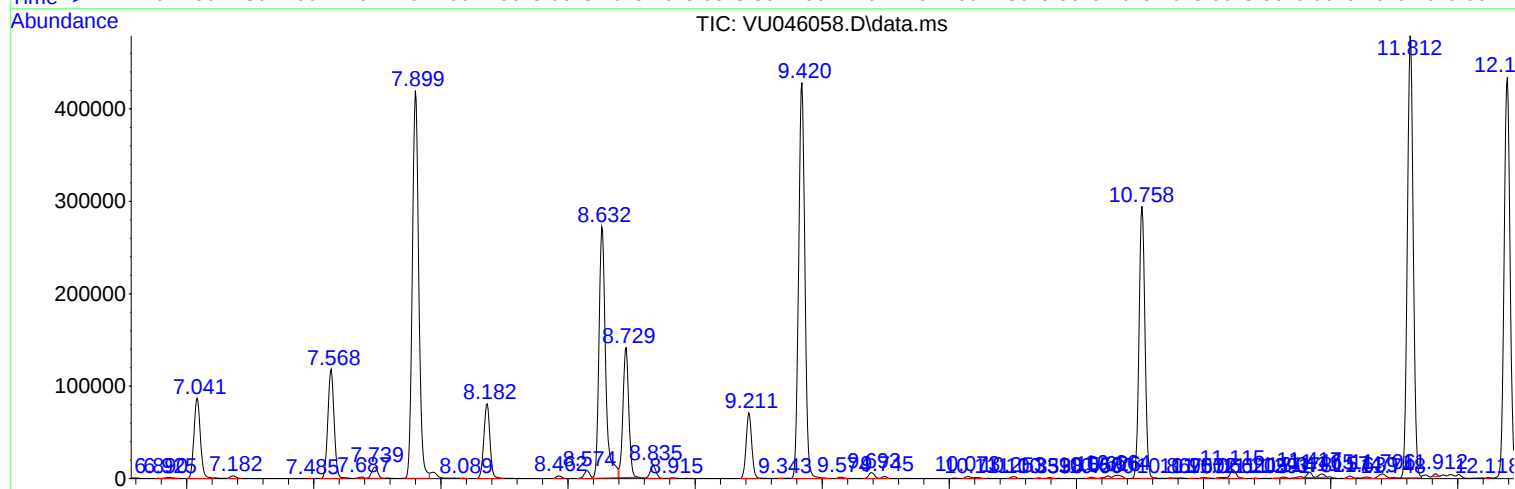
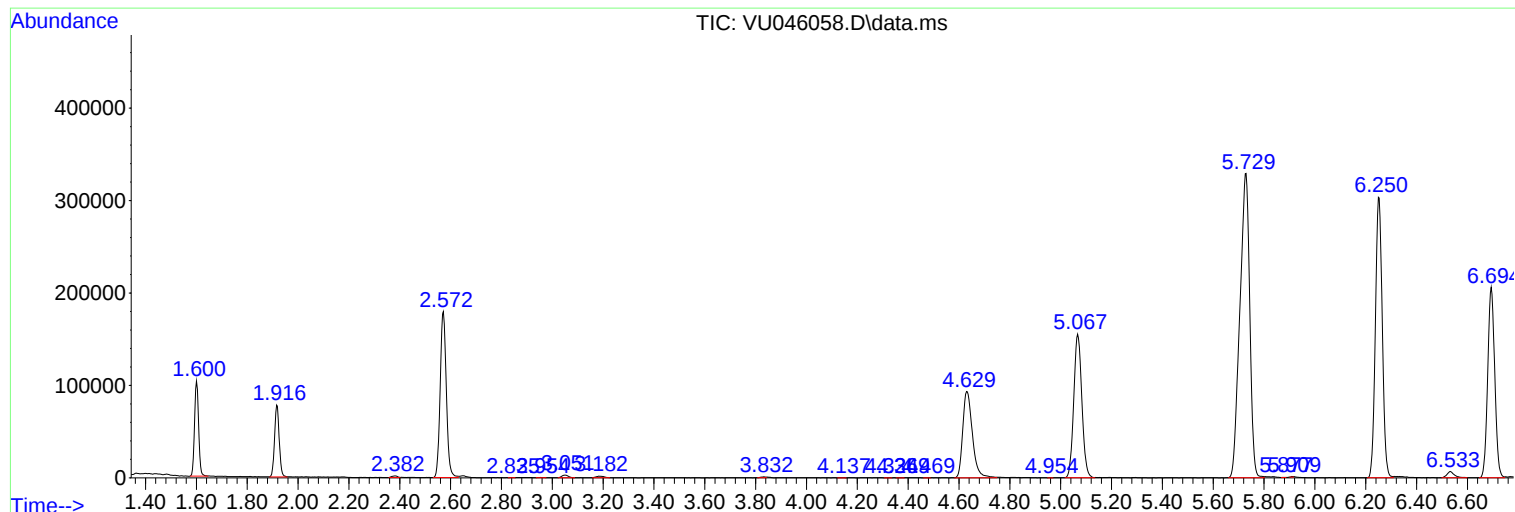
Sum of corrected areas: 7893697

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Instrument :
MSVOA_U
ClientSampleId :
VLEB128

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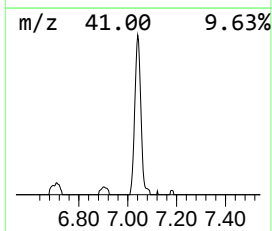
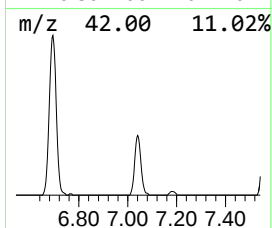
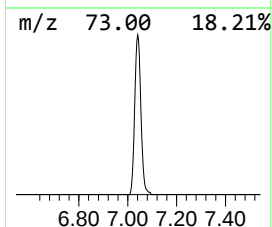
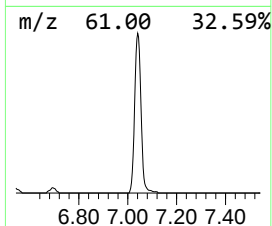
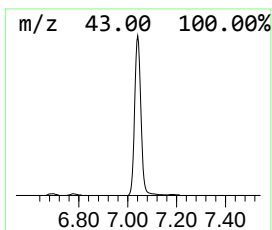
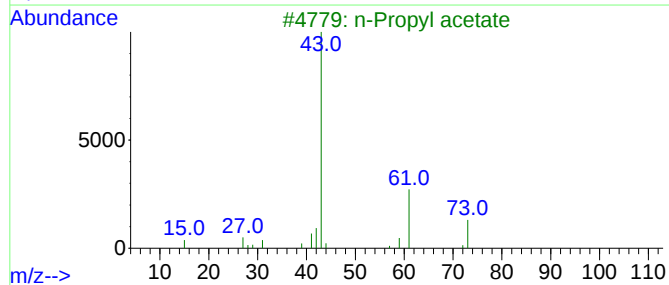
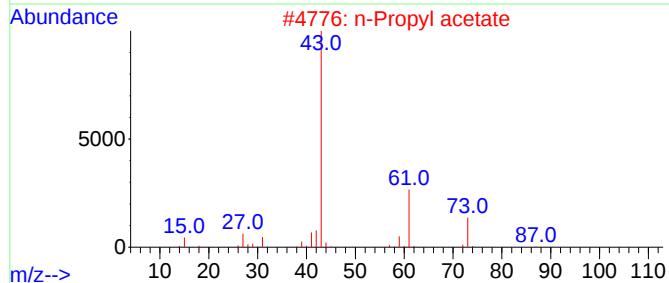
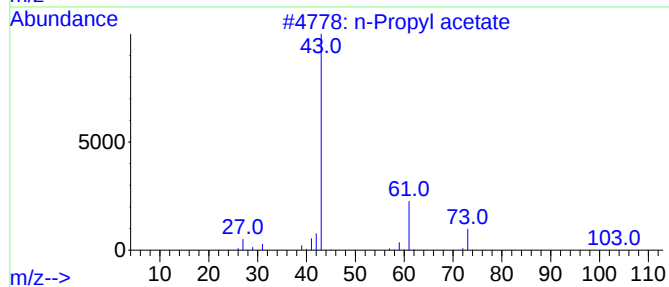
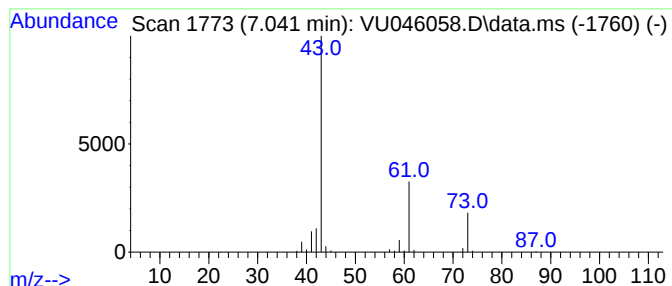
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	13.32 ug/L	152627	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	83
2	n-Propyl acetate			102	C5H10O2	000109-60-4	83
3	n-Propyl acetate			102	C5H10O2	000109-60-4	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	50
5	Propanal, 2,3-dihydroxy-, (S)-			90	C3H6O3	000497-09-6	36



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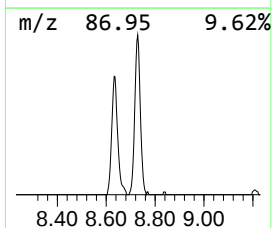
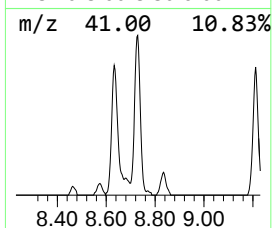
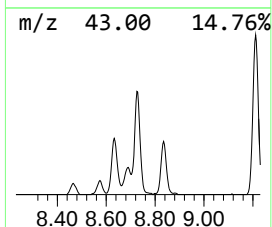
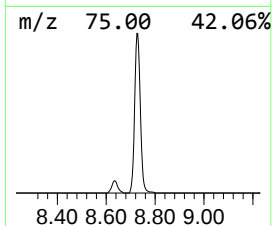
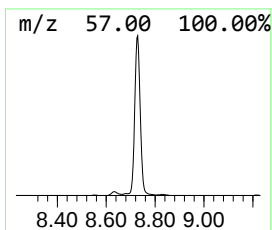
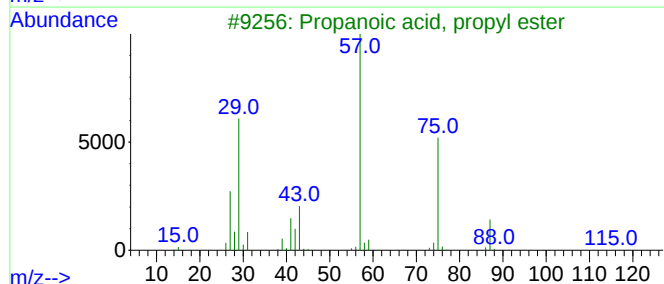
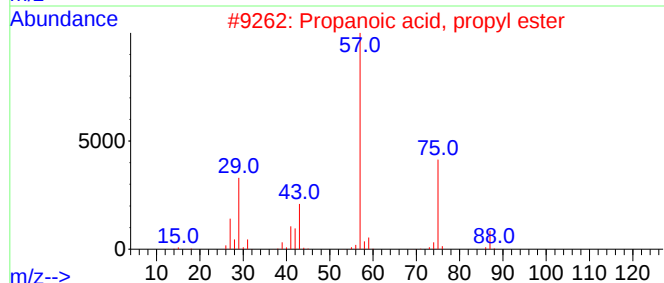
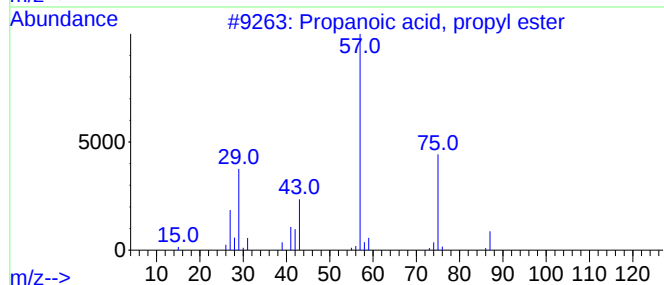
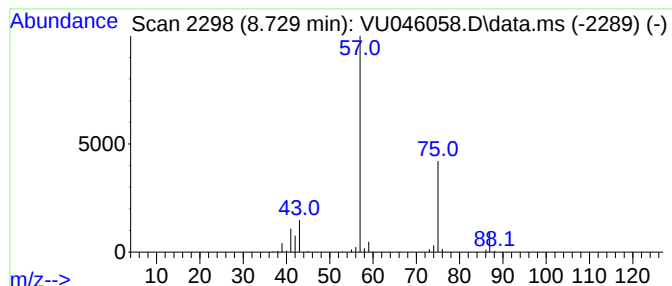
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Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	15.17 ug/L	220087	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74



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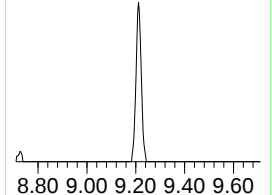
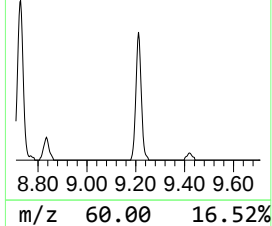
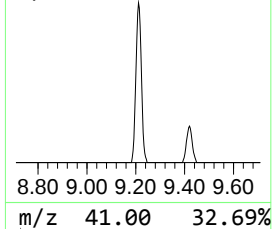
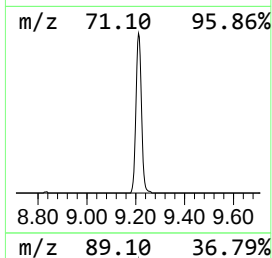
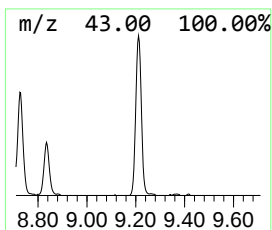
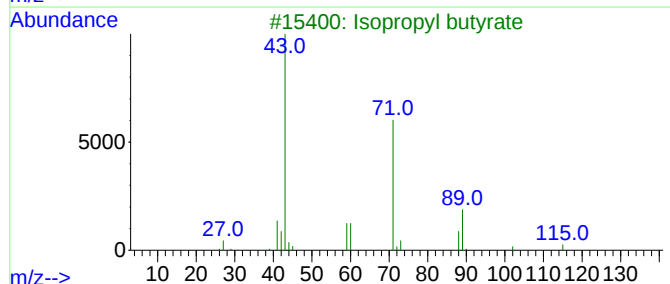
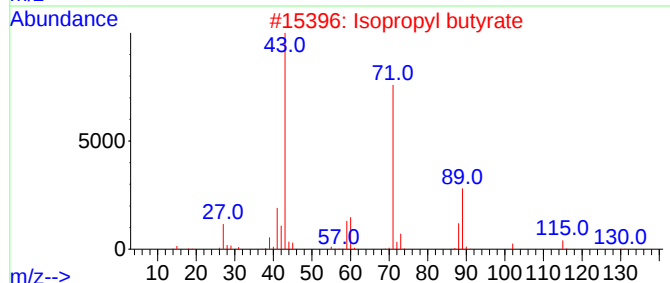
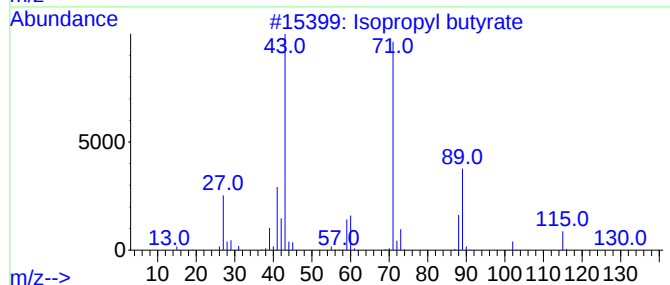
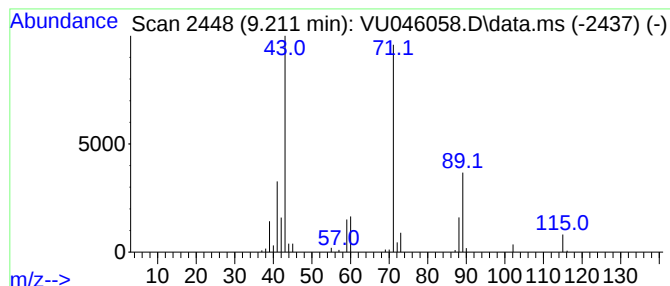
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	7.53 ug/L	109261	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
5			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120221\
Data File : VU046058.D
Acq On : 02 Dec 2021 17:27
Operator : SY/MD
Sample : PB141128TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB128

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.041	13.3	ug/L	152627	1	6.253	572752	50.0
Propanoic acid,...	8.729	15.2	ug/L	220087	2	9.420	725292	50.0
Isopropyl butyrate	9.211	7.5	ug/L	109261	2	9.420	725292	50.0