

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
 Data File : VU046117.D
 Acq On : 06 Dec 2021 17:34
 Operator : SY/MD
 Sample : M4938-07 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8E3

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: VU046117.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	94	rVB	98404	107523	13.30%	1.679%
2	1.916	170	179	197	rVB	68960	87726	10.85%	1.370%
3	2.243	279	281	284	rVB	439	174	0.02%	0.003%
4	2.501	358	361	364	rBV3	386	278	0.03%	0.004%
5	2.571	370	383	402	rBV	170817	285476	35.32%	4.458%
6	2.713	423	427	428	rBV	190	142	0.02%	0.002%
7	2.796	447	453	462	rVB3	727	1151	0.14%	0.018%
8	2.954	497	502	503	rBV	215	181	0.02%	0.003%
9	3.051	523	532	542	rVB3	5540	9934	1.23%	0.155%
10	3.192	565	576	588	rBV2	2108	4713	0.58%	0.074%
11	3.260	594	597	602	rVB2	200	160	0.02%	0.002%
12	3.359	624	628	631	rBV3	362	263	0.03%	0.004%
13	3.780	757	759	765	rVB2	165	153	0.02%	0.002%
14	3.890	790	793	795	rBV	199	157	0.02%	0.002%
15	4.198	886	889	896	rVV	192	139	0.02%	0.002%
16	4.311	921	924	927	rBV	180	163	0.02%	0.003%
17	4.407	950	954	956	rBV	248	140	0.02%	0.002%
18	4.555	996	1000	1003	rBV2	170	130	0.02%	0.002%
19	4.629	1007	1023	1047	rBV	81286	205427	25.41%	3.208%
20	4.774	1064	1068	1069	rBV	198	131	0.02%	0.002%
21	4.857	1086	1094	1097	rBV2	275	399	0.05%	0.006%
22	5.067	1142	1159	1183	rBV	137404	315938	39.09%	4.934%
23	5.150	1183	1185	1188	rVB3	349	187	0.02%	0.003%
24	5.295	1224	1230	1233	rBV2	337	470	0.06%	0.007%
25	5.420	1266	1269	1280	rVB	133	144	0.02%	0.002%
26	5.468	1280	1284	1289	rBV2	165	166	0.02%	0.003%
27	5.729	1343	1365	1384	rBV2	299839	808313	100.00%	12.623%
28	5.919	1420	1424	1435	rVB3	1240	1712	0.21%	0.027%
29	5.967	1435	1439	1441	rBV	262	251	0.03%	0.004%
30	6.012	1447	1453	1455	rBV2	216	223	0.03%	0.003%
31	6.034	1458	1460	1464	rBV	179	186	0.02%	0.003%
32	6.253	1512	1528	1547	rBV	225915	427058	52.83%	6.669%
33	6.539	1606	1617	1631	rVB5	10852	21384	2.65%	0.334%
34	6.693	1651	1665	1684	rBV	184895	355242	43.95%	5.547%
35	6.861	1712	1717	1720	rBV	218	232	0.03%	0.004%
36	6.928	1731	1738	1744	rBV2	774	1304	0.16%	0.020%

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

37	7.041	1761	1773	1790	rBV	41898	73286	9.07%	1.144%
38	7.179	1812	1816	1820	rBV3	478	445	0.06%	0.007%
39	7.369	1871	1875	1878	rVV	130	136	0.02%	0.002%
40	7.568	1922	1937	1959	rBV	106673	185558	22.96%	2.898%
41	7.661	1963	1966	1969	rBV2	247	186	0.02%	0.003%
42	7.681	1969	1972	1976	rVB	333	208	0.03%	0.003%
43	7.738	1980	1990	1999	rBV2	6854	10573	1.31%	0.165%
44	7.899	2027	2040	2056	rBV	386546	669488	82.83%	10.455%
45	8.182	2116	2128	2145	rBV	72316	120945	14.96%	1.889%
46	8.304	2163	2166	2173	rVB2	315	335	0.04%	0.005%
47	8.468	2206	2217	2221	rBV4	916	1233	0.15%	0.019%
48	8.555	2235	2244	2248	rBV4	3255	4935	0.61%	0.077%
49	8.635	2256	2269	2290	rBV	244574	423950	52.45%	6.620%
50	8.729	2290	2298	2313	rVB	35412	56182	6.95%	0.877%
51	8.832	2324	2330	2343	rVB2	2561	3869	0.48%	0.060%
52	8.912	2348	2355	2363	rBV4	903	1373	0.17%	0.021%
53	9.163	2428	2433	2439	rVV3	460	465	0.06%	0.007%
54	9.211	2439	2448	2459	rVB	13469	20064	2.48%	0.313%
55	9.420	2499	2513	2538	rBV	323140	538085	66.57%	8.403%
56	9.571	2552	2560	2566	rVB3	810	1057	0.13%	0.017%
57	9.629	2574	2578	2582	rVV2	176	129	0.02%	0.002%
58	9.693	2588	2598	2608	rVV2	1416	2410	0.30%	0.038%
59	9.748	2611	2615	2619	rVB2	207	173	0.02%	0.003%
60	9.816	2632	2636	2639	rBV2	158	144	0.02%	0.002%
61	9.934	2671	2673	2678	rVB	219	134	0.02%	0.002%
62	10.037	2701	2705	2708	rVB	204	171	0.02%	0.003%
63	10.095	2717	2723	2724	rBV	432	367	0.05%	0.006%
64	10.115	2725	2729	2732	rVB3	721	608	0.08%	0.009%
65	10.253	2768	2772	2774	rBV	226	178	0.02%	0.003%
66	10.397	2814	2817	2823	rBV2	245	341	0.04%	0.005%
67	10.484	2838	2844	2850	rVB2	463	561	0.07%	0.009%
68	10.668	2894	2901	2902	rBV2	1812	1402	0.17%	0.022%
69	10.758	2917	2929	2947	rBV	266428	420170	51.98%	6.561%
70	10.996	3000	3003	3004	rBV	253	131	0.02%	0.002%
71	11.037	3013	3016	3019	rBV	192	176	0.02%	0.003%
72	11.092	3026	3033	3037	rBV3	613	668	0.08%	0.010%
73	11.298	3095	3097	3098	rBV	263	128	0.02%	0.002%
74	11.378	3118	3122	3125	rBV2	223	182	0.02%	0.003%
75	11.459	3139	3147	3148	rBV3	1724	1733	0.21%	0.027%
76	11.696	3217	3221	3223	rBV3	595	434	0.05%	0.007%

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

77	11.745	3232	3236	3245	rVB3	915	1075	0.13%	0.017%
78	11.812	3245	3257	3273	rBV	364113	571522	70.71%	8.925%
79	11.950	3295	3300	3302	rBV3	478	453	0.06%	0.007%
80	11.976	3302	3308	3315	rVB4	1531	2095	0.26%	0.033%
81	12.082	3339	3341	3347	rVB2	204	157	0.02%	0.002%
82	12.195	3360	3376	3393	rVB	396146	632968	78.31%	9.884%
83	12.327	3413	3417	3425	rVB4	799	939	0.12%	0.015%
84	12.458	3455	3458	3462	rVV2	180	158	0.02%	0.002%
85	12.526	3476	3479	3483	rVB2	252	187	0.02%	0.003%
86	12.893	3591	3593	3599	rBV	162	133	0.02%	0.002%
87	13.217	3690	3694	3695	rBV2	838	485	0.06%	0.008%
88	13.497	3777	3781	3785	rBV	180	179	0.02%	0.003%
89	13.847	3882	3890	3897	rVB4	1556	2178	0.27%	0.034%
90	13.963	3921	3926	3927	rBV2	261	214	0.03%	0.003%
91	14.089	3956	3965	3976	rVB	3303	4583	0.57%	0.072%
92	14.333	4034	4041	4049	rBV3	1545	1928	0.24%	0.030%
93	14.397	4059	4061	4065	rBV2	237	164	0.02%	0.003%
94	14.481	4085	4087	4089	rBV	273	139	0.02%	0.002%
95	14.513	4089	4097	4103	rVB2	368	521	0.06%	0.008%
96	14.577	4112	4117	4119	rBV2	619	603	0.07%	0.009%
97	15.037	4258	4260	4263	rBV2	320	169	0.02%	0.003%
98	15.224	4313	4318	4327	rVB3	1325	2198	0.27%	0.034%
99	15.407	4371	4375	4377	rBV4	624	392	0.05%	0.006%
100	16.317	4656	4658	4661	rBV2	431	269	0.03%	0.004%

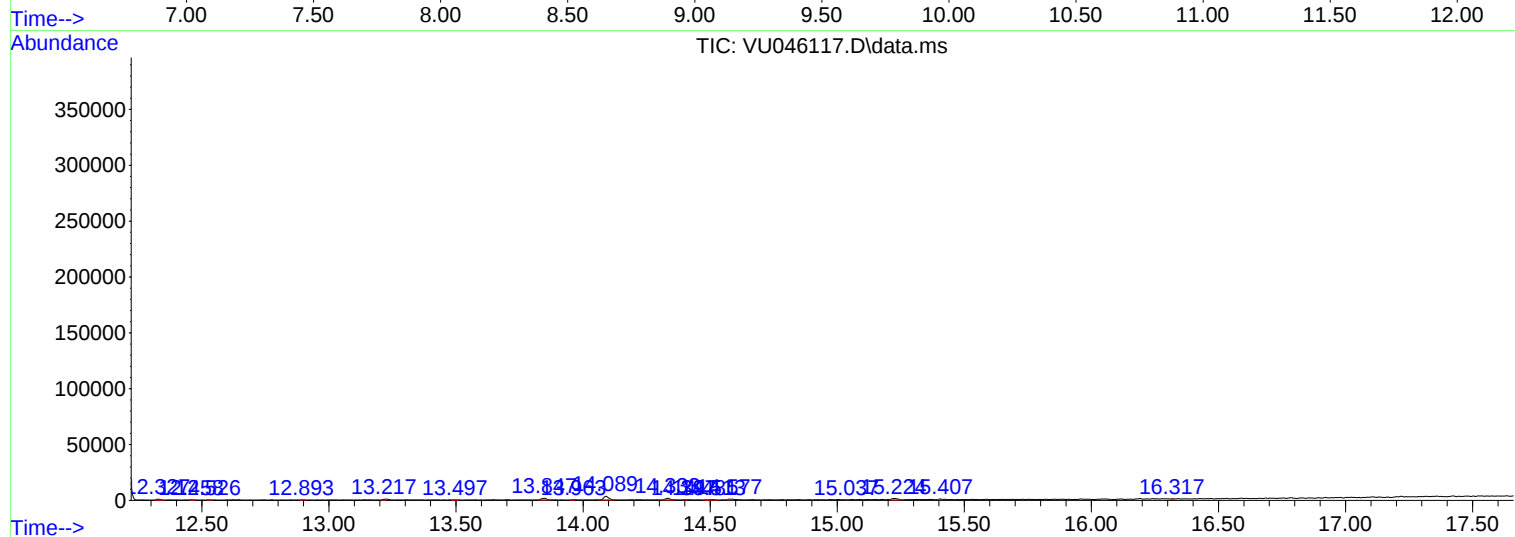
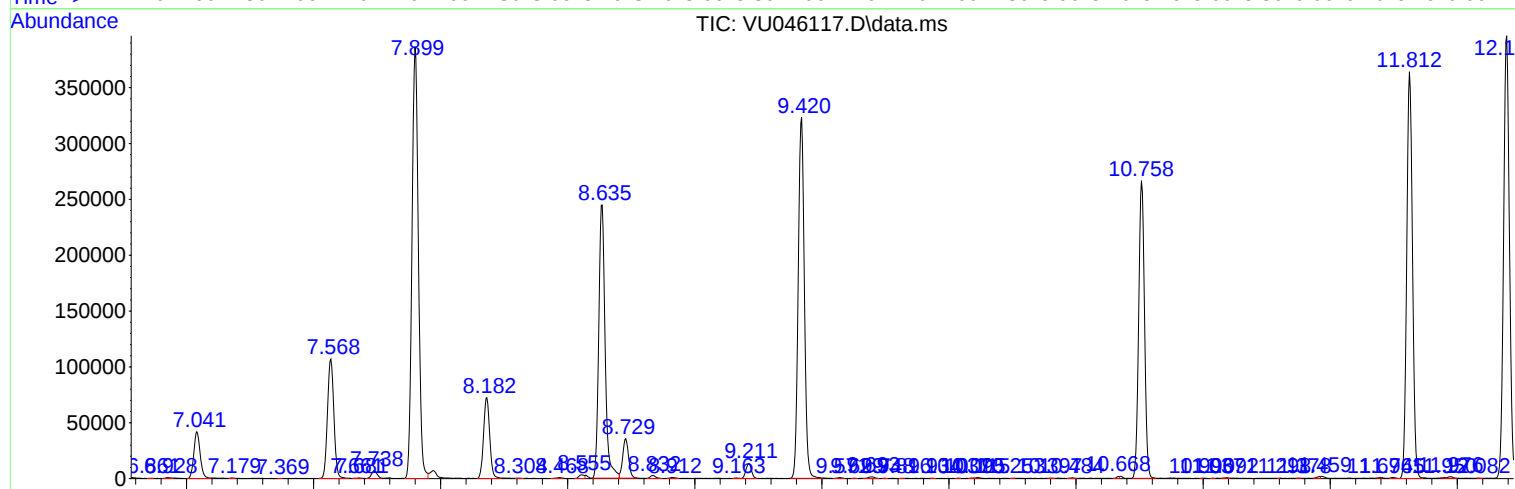
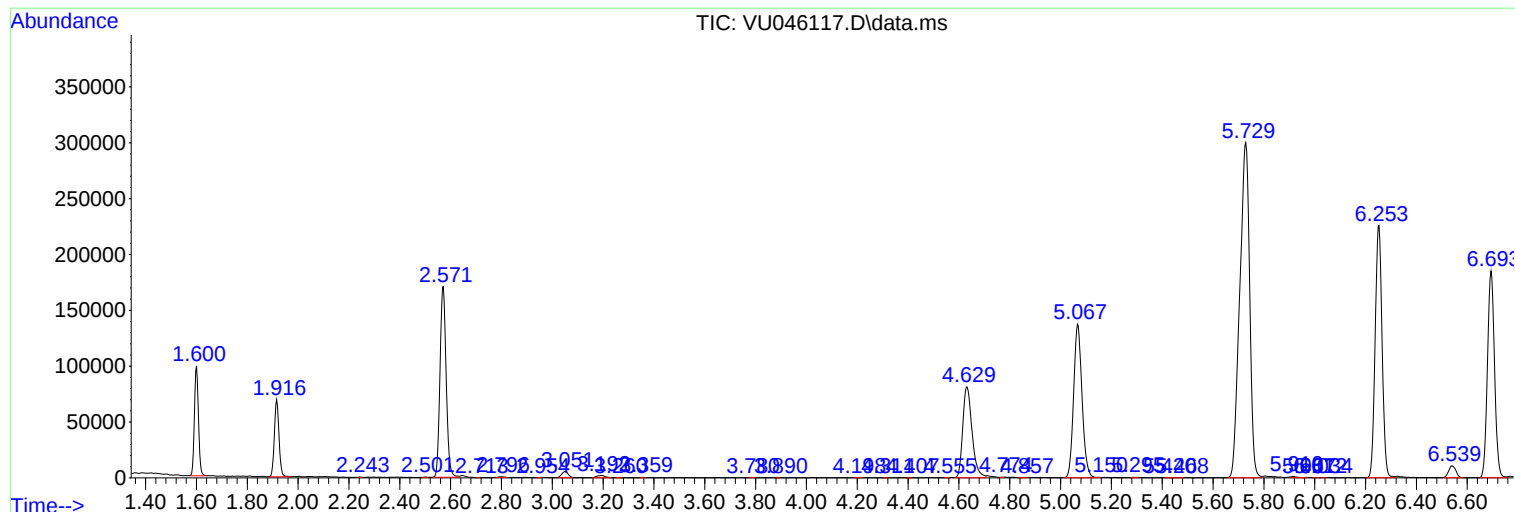
Sum of corrected areas: 6403692

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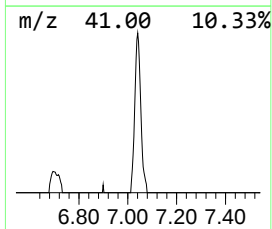
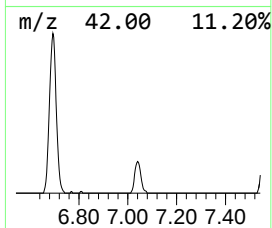
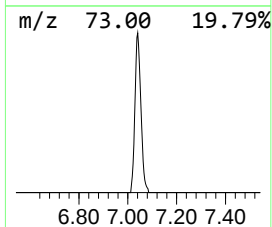
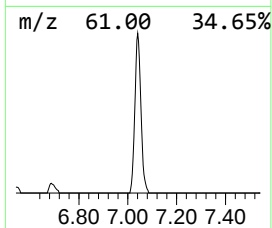
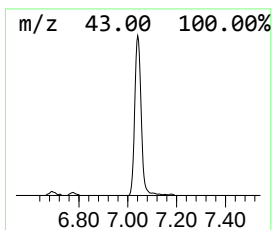
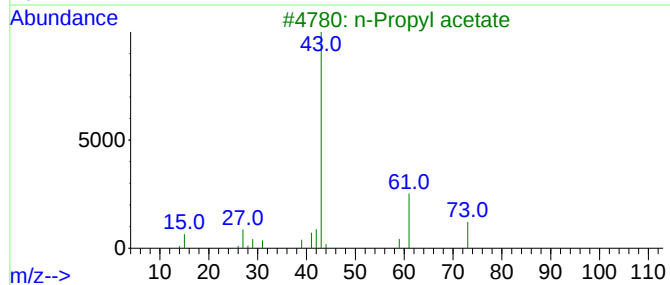
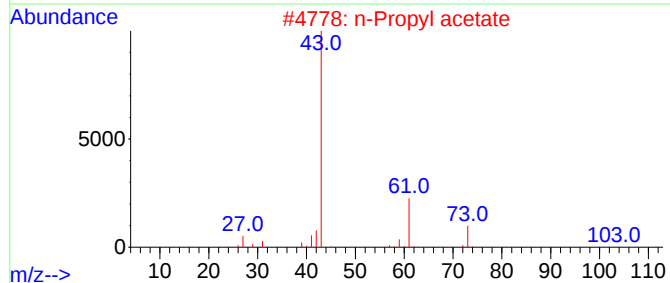
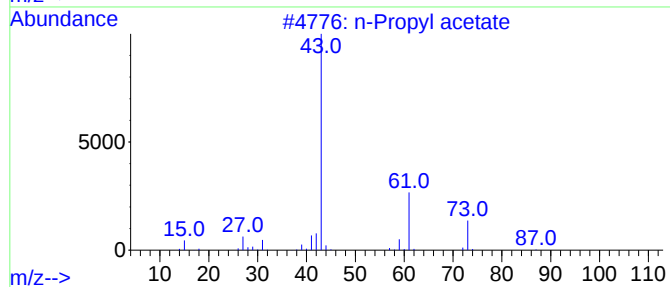
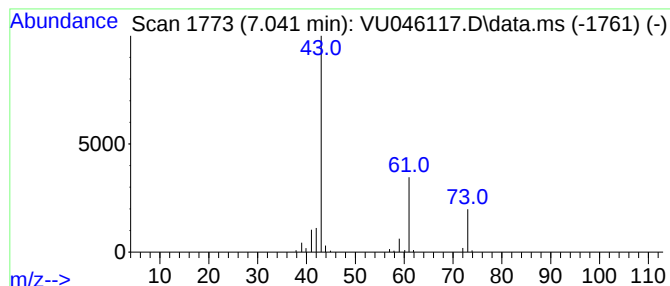
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	8.58 ug/L	73286	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	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	Propanal, 2,3-dihydroxy-, (S)-			90	C3H6O3	000497-09-6	38



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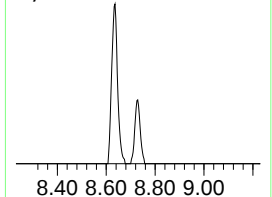
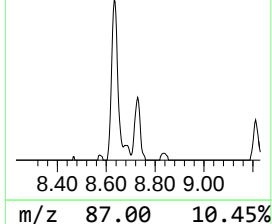
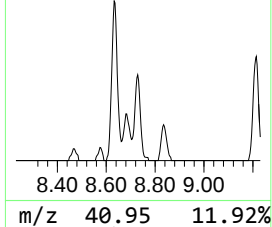
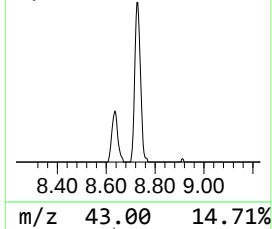
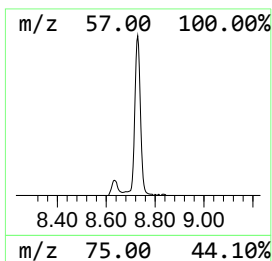
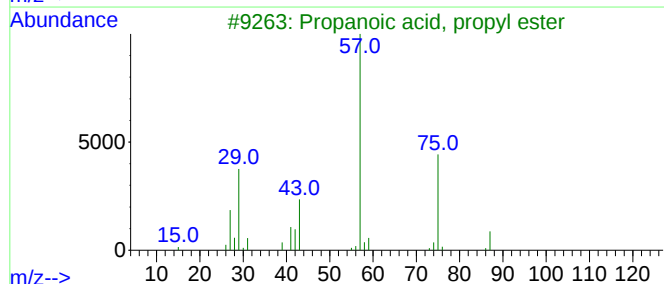
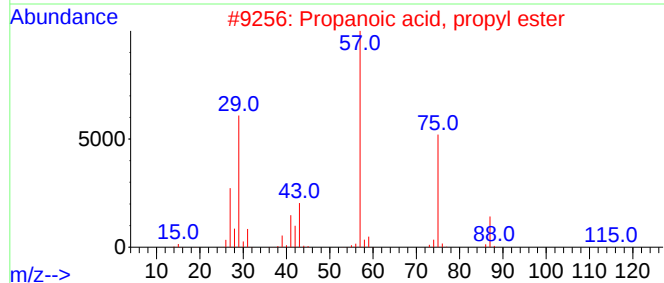
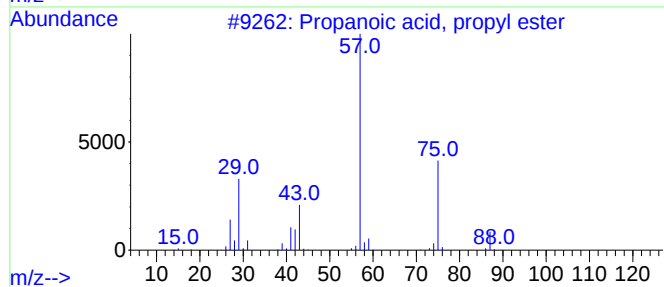
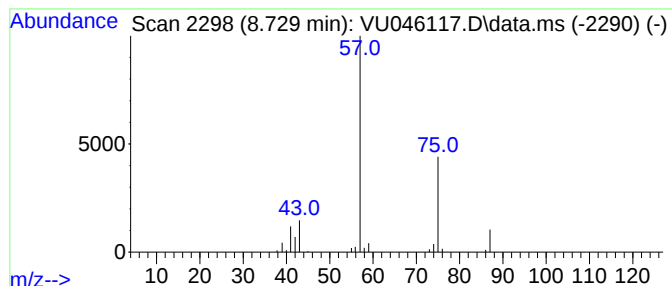
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	5.22 ug/L	56182	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56
5			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	9



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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	8.6	ug/L	73286	1	6.253	427058	50.0
Propanoic acid,...	8.729	5.2	ug/L	56182	2	9.420	538085	50.0