

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049358.D
 Acq On : 22 Jun 2022 17:43
 Operator : SY/MD
 Sample : N3392-12 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEY7

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\SFAMULM061022WMA.M
 Title : VOC Analysis

Signal : TIC: VU049358.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	40	45	49	rBV4	2609	3087	0.42%	0.045%
2	1.597	73	80	91	rBV	66073	75479	10.20%	1.097%
3	1.903	168	175	193	rVB	56381	78257	10.57%	1.137%
4	2.565	369	381	393	rBV	111384	180300	24.35%	2.620%
5	2.633	395	402	415	rVB	6159	11230	1.52%	0.163%
6	2.787	445	450	455	rBV3	826	1242	0.17%	0.018%
7	2.951	494	501	502	rBV	732	719	0.10%	0.010%
8	3.047	520	531	539	rBV3	3111	5930	0.80%	0.086%
9	3.186	558	574	591	rBV	20317	48953	6.61%	0.711%
10	3.269	598	600	603	rVB2	491	252	0.03%	0.004%
11	3.437	649	652	656	rVB2	335	232	0.03%	0.003%
12	3.575	691	695	696	rBV	672	495	0.07%	0.007%
13	3.822	768	772	774	rBV	267	230	0.03%	0.003%
14	3.845	774	779	782	rBV3	206	227	0.03%	0.003%
15	3.990	820	824	827	rBV3	301	236	0.03%	0.003%
16	4.215	891	894	899	rVB2	264	278	0.04%	0.004%
17	4.237	899	901	906	rBV	305	301	0.04%	0.004%
18	4.334	927	931	936	rBV	213	234	0.03%	0.003%
19	4.562	998	1002	1005	rBV3	250	227	0.03%	0.003%
20	4.626	1008	1022	1066	rBV	121715	329201	44.47%	4.785%
21	4.813	1077	1080	1093	rVB4	1225	1863	0.25%	0.027%
22	4.922	1112	1114	1121	rVB2	361	306	0.04%	0.004%
23	4.954	1121	1124	1129	rVB2	329	356	0.05%	0.005%
24	4.980	1129	1132	1134	rBV2	375	229	0.03%	0.003%
25	4.996	1134	1137	1141	rVB3	476	353	0.05%	0.005%
26	5.063	1141	1158	1177	rBV	145295	315000	42.55%	4.578%
27	5.289	1224	1228	1233	rBV3	436	462	0.06%	0.007%
28	5.568	1309	1315	1317	rBV2	290	280	0.04%	0.004%
29	5.626	1330	1333	1339	rVB	274	263	0.04%	0.004%
30	5.723	1339	1363	1385	rBV2	266450	740313	100.00%	10.759%
31	5.912	1410	1422	1435	rBV2	7456	14947	2.02%	0.217%
32	6.125	1484	1488	1492	rBV4	1061	1155	0.16%	0.017%
33	6.247	1513	1526	1552	rBV	297525	565470	76.38%	8.218%
34	6.523	1606	1612	1614	rBV5	1510	1494	0.20%	0.022%
35	6.597	1631	1635	1638	rVB2	582	389	0.05%	0.006%
36	6.623	1638	1643	1644	rBV2	609	431	0.06%	0.006%

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 Title : VOC Analysis

37	6.690	1649	1664	1680	rBV	194678	370808	50.09%	5.389%
38	6.813	1697	1702	1707	rVB5	1044	1229	0.17%	0.018%
39	6.880	1719	1723	1726	rVV4	387	309	0.04%	0.004%
40	6.928	1730	1738	1758	rVB	3677	8266	1.12%	0.120%
41	7.041	1760	1773	1799	rBV	86994	162795	21.99%	2.366%
42	7.182	1813	1817	1830	rVB6	1865	3135	0.42%	0.046%
43	7.372	1873	1876	1881	rVB3	391	317	0.04%	0.005%
44	7.436	1894	1896	1902	rVB3	371	250	0.03%	0.004%
45	7.491	1908	1913	1918	rVB2	547	404	0.05%	0.006%
46	7.565	1921	1936	1958	rBV	97558	176177	23.80%	2.561%
47	7.694	1966	1976	1981	rBV5	1083	1682	0.23%	0.024%
48	7.739	1981	1990	2001	rBV2	15402	26703	3.61%	0.388%
49	7.896	2026	2039	2060	rBV	298978	524675	70.87%	7.625%
50	8.083	2092	2097	2099	rBV2	360	242	0.03%	0.004%
51	8.179	2110	2127	2142	rBV2	72087	145891	19.71%	2.120%
52	8.327	2170	2173	2179	rVB3	576	470	0.06%	0.007%
53	8.465	2203	2216	2232	rVB3	17190	29026	3.92%	0.422%
54	8.526	2232	2235	2237	rBV2	360	242	0.03%	0.004%
55	8.571	2237	2249	2256	rBV6	3956	7715	1.04%	0.112%
56	8.636	2256	2269	2289	rVV	342074	617925	83.47%	8.981%
57	8.726	2290	2297	2313	rVB	52166	86348	11.66%	1.255%
58	8.835	2323	2331	2346	rVB2	17781	29602	4.00%	0.430%
59	9.108	2414	2416	2424	rVV2	271	341	0.05%	0.005%
60	9.211	2437	2448	2462	rVV	58586	93452	12.62%	1.358%
61	9.276	2466	2468	2471	rVV3	691	517	0.07%	0.008%
62	9.327	2481	2484	2489	rVB	412	290	0.04%	0.004%
63	9.366	2489	2496	2499	rBV4	1177	1495	0.20%	0.022%
64	9.417	2499	2512	2528	rBV	400283	656115	88.63%	9.536%
65	9.739	2608	2612	2615	rBV	349	274	0.04%	0.004%
66	9.774	2617	2623	2631	rVB	295	401	0.05%	0.006%
67	9.832	2637	2641	2644	rVB2	334	260	0.04%	0.004%
68	9.915	2663	2667	2668	rBV	538	305	0.04%	0.004%
69	10.044	2703	2707	2710	rBV2	277	249	0.03%	0.004%
70	10.073	2710	2716	2730	rVB4	2824	4151	0.56%	0.060%
71	10.131	2730	2734	2737	rBV	283	266	0.04%	0.004%
72	10.349	2798	2802	2805	rBV2	245	238	0.03%	0.003%
73	10.484	2842	2844	2851	rVB3	262	262	0.04%	0.004%
74	10.542	2860	2862	2869	rVB4	432	433	0.06%	0.006%
75	10.755	2916	2928	2949	rVV	294860	478398	64.62%	6.953%
76	10.912	2975	2977	2983	rVB2	316	323	0.04%	0.005%

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 Title : VOC Analysis

77	11.092	3028	3033	3036	rBV2	360	291	0.04%	0.004%
78	11.124	3039	3043	3049	rVB2	398	442	0.06%	0.006%
79	11.166	3050	3056	3059	rBV2	465	382	0.05%	0.006%
80	11.385	3120	3124	3130	rVB3	288	327	0.04%	0.005%
81	11.417	3130	3134	3137	rBV2	302	260	0.04%	0.004%
82	11.546	3171	3174	3180	rBV	241	264	0.04%	0.004%
83	11.623	3195	3198	3201	rBV	282	265	0.04%	0.004%
84	11.812	3241	3257	3277	rBV	355029	574121	77.55%	8.344%
85	11.928	3290	3293	3296	rVB3	466	390	0.05%	0.006%
86	12.118	3347	3352	3353	rBV2	252	227	0.03%	0.003%
87	12.192	3363	3375	3390	rBV	301741	486142	65.67%	7.065%
88	12.446	3449	3454	3459	rBV3	379	516	0.07%	0.007%
89	12.774	3550	3556	3558	rBV3	654	576	0.08%	0.008%
90	12.967	3613	3616	3619	rBV	389	262	0.04%	0.004%
91	13.327	3724	3728	3733	rBV3	374	400	0.05%	0.006%
92	13.510	3782	3785	3790	rBV	394	380	0.05%	0.006%
93	13.816	3877	3880	3884	rVB3	356	273	0.04%	0.004%
94	13.883	3899	3901	3904	rBV	365	273	0.04%	0.004%
95	13.938	3913	3918	3921	rBV2	273	281	0.04%	0.004%
96	14.481	4084	4087	4089	rBV2	472	267	0.04%	0.004%
97	14.738	4165	4167	4170	rBV2	465	294	0.04%	0.004%
98	14.851	4199	4202	4205	rBV	447	402	0.05%	0.006%
99	15.555	4418	4421	4424	rBV2	432	350	0.05%	0.005%
100	15.996	4555	4558	4565	rVB4	755	776	0.10%	0.011%

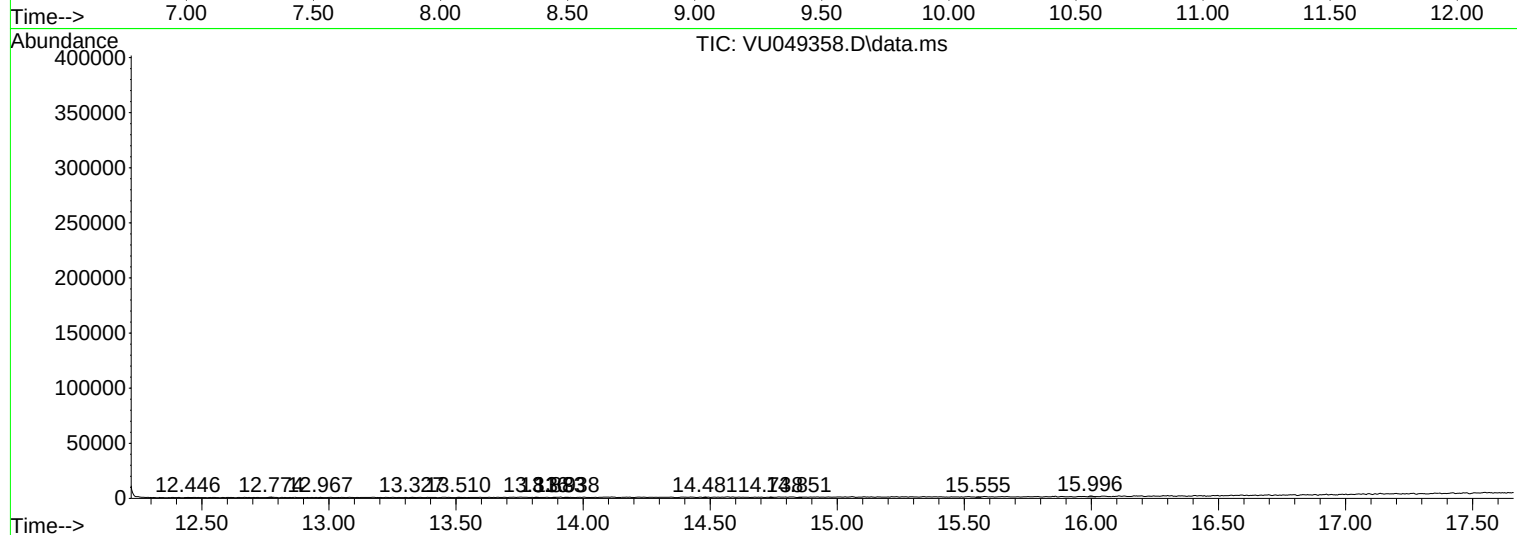
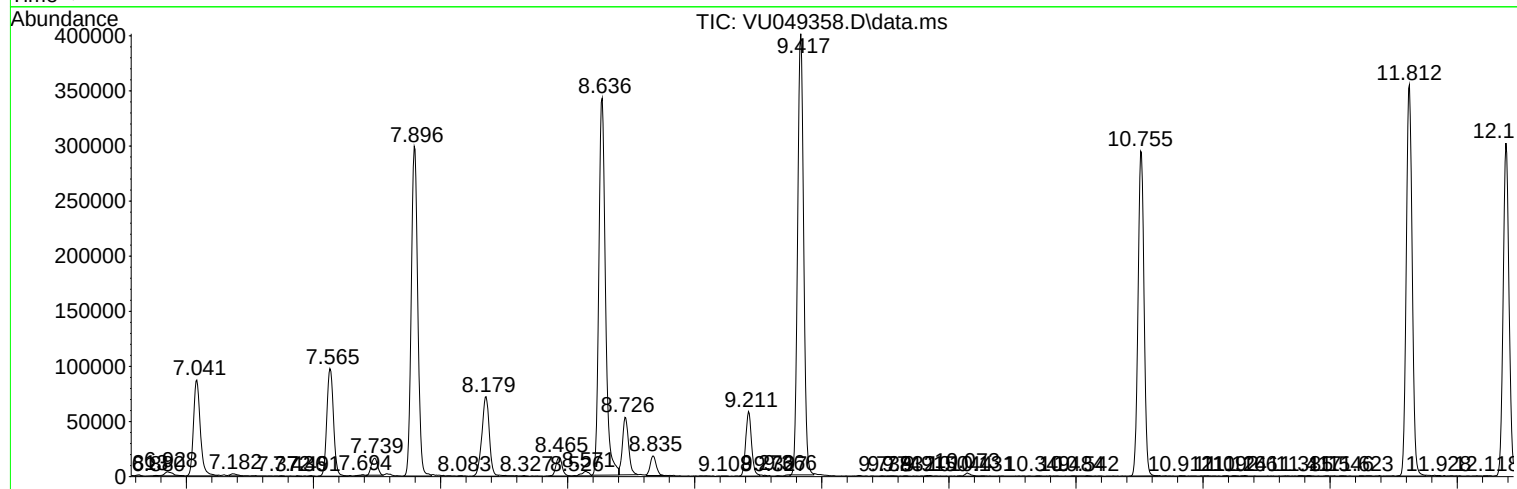
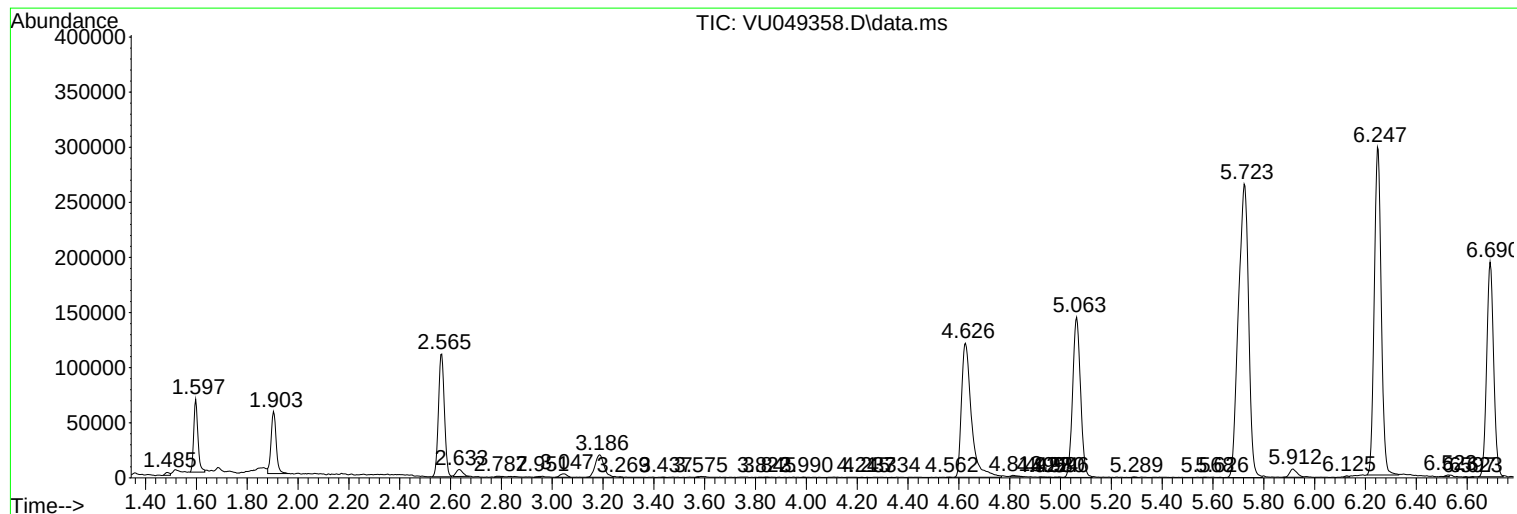
Sum of corrected areas: 6880563

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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



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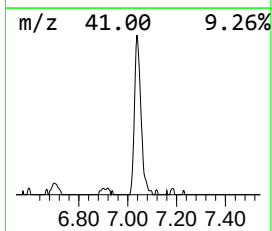
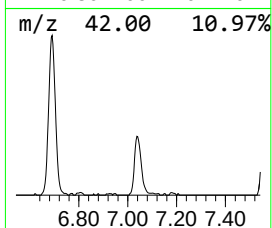
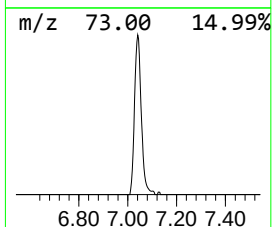
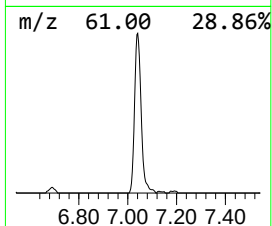
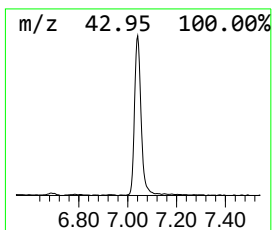
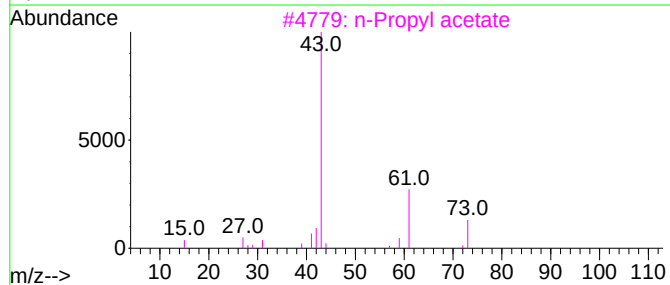
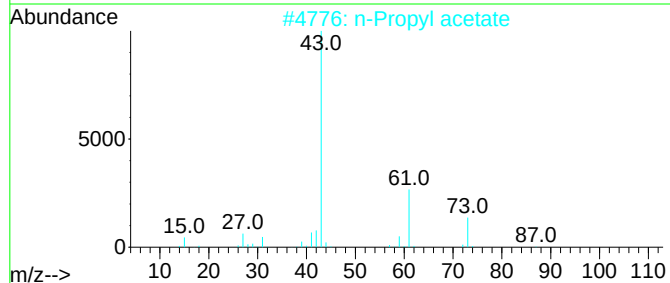
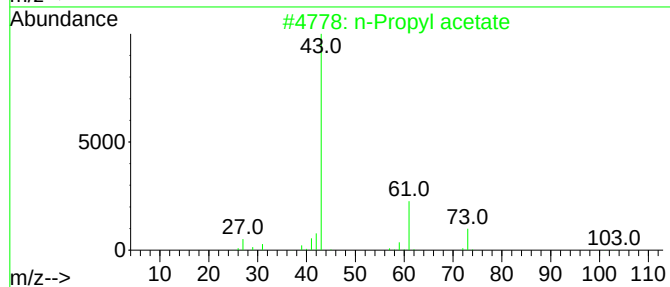
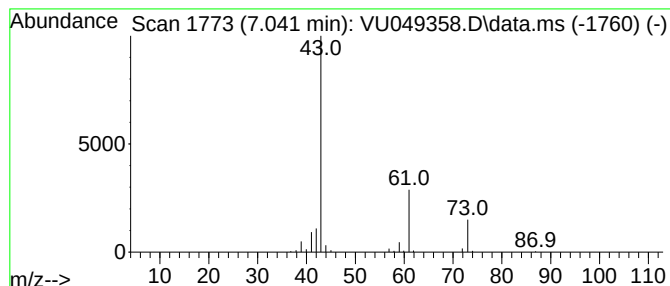
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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	14.39 ug/L	162795	1,4-Difluorobenzene	6.250

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	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	78
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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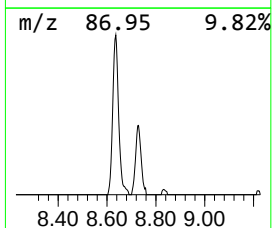
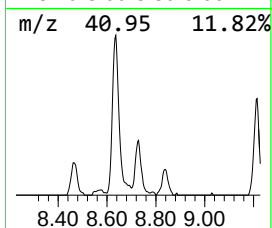
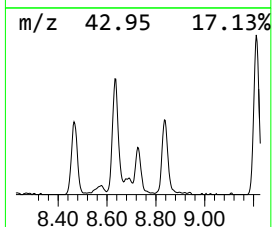
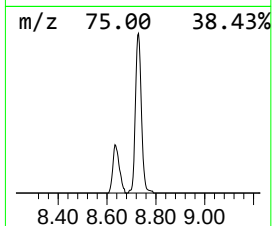
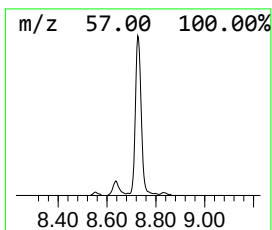
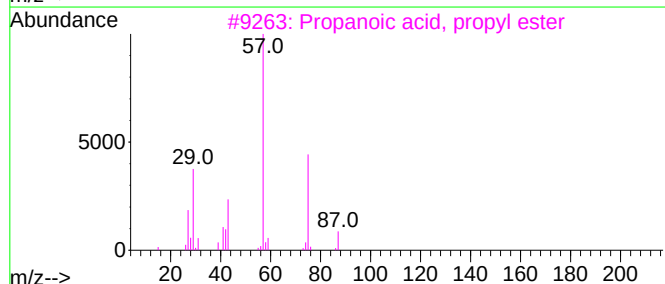
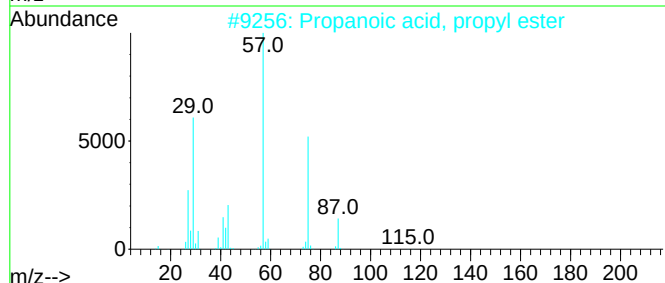
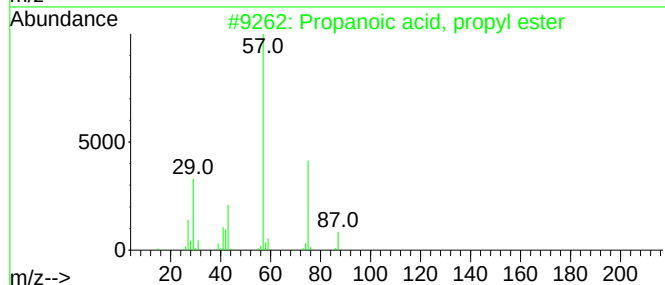
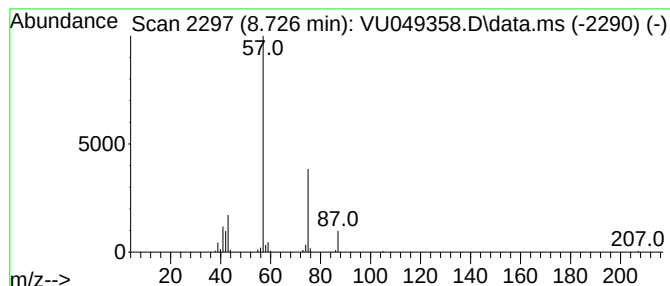
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	6.58 ug/L	86348	Chlorobenzene-d5	9.417

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	78
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72



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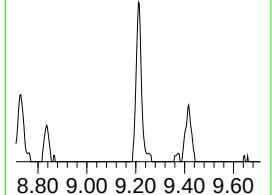
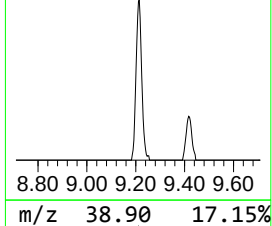
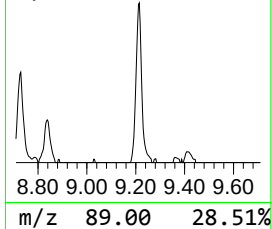
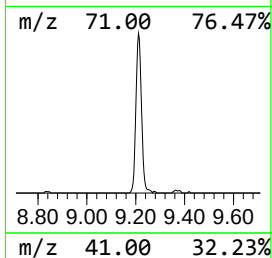
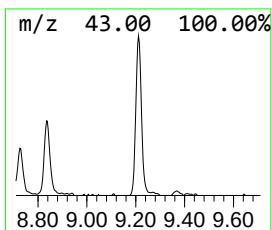
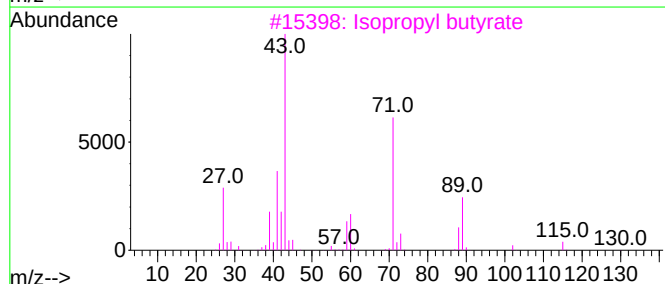
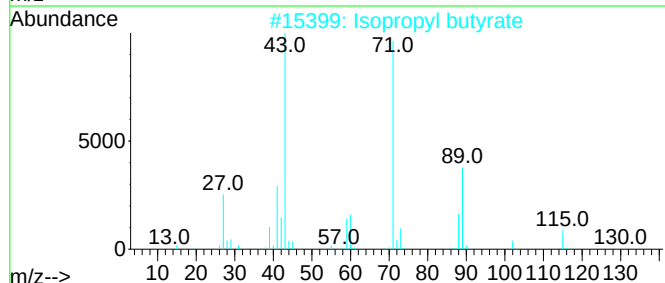
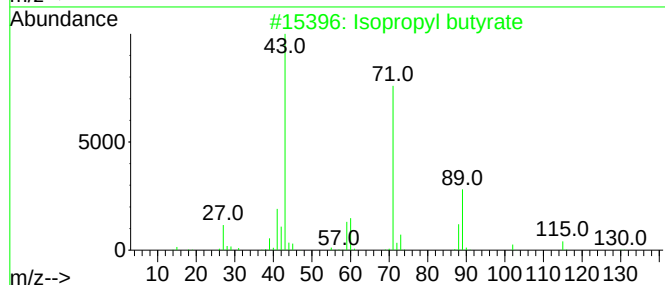
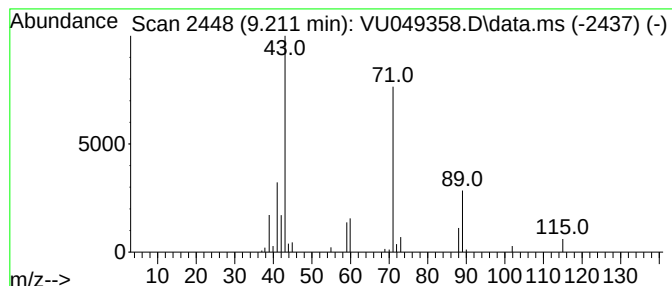
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	7.12 ug/L	93452	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049358.D
Acq On : 22 Jun 2022 17:43
Operator : SY/MD
Sample : N3392-12 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.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	14.4	ug/L	162795	1	6.250	565470	50.0
Propanoic acid,...	8.726	6.6	ug/L	86348	2	9.417	656115	50.0
Isopropyl butyrate	9.211	7.1	ug/L	93452	2	9.417	656115	50.0