

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042722\
 Data File : VU048309.D
 Acq On : 27 Apr 2022 13:08
 Operator : SY/MD
 Sample : N2542-02 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXER8

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\SFAMULM042522WMA.M

Title : VOC Analysis

Signal : TIC: VU048309.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	51	rBV3	4419	5342	0.33%	0.042%
2	1.600	73	81	100	rBV	188301	241705	14.95%	1.909%
3	1.887	163	170	192	rVB	129073	203545	12.59%	1.608%
4	2.562	368	380	396	rBV	336541	544994	33.72%	4.305%
5	2.739	431	435	439	rBV2	502	481	0.03%	0.004%
6	2.790	439	451	452	rBV6	1037	1474	0.09%	0.012%
7	2.906	482	487	491	rVB3	265	284	0.02%	0.002%
8	2.938	492	497	499	rBV2	404	390	0.02%	0.003%
9	2.993	511	514	518	rBV2	325	272	0.02%	0.002%
10	3.044	520	530	549	rBV	13363	27528	1.70%	0.217%
11	3.182	559	573	599	rBV	24411	60809	3.76%	0.480%
12	3.401	638	641	643	rBV	184	162	0.01%	0.001%
13	3.568	691	693	698	rVB	339	182	0.01%	0.001%
14	3.597	698	702	706	rBV2	165	153	0.01%	0.001%
15	3.655	716	720	727	rBV2	294	322	0.02%	0.003%
16	3.825	769	773	776	rVB2	312	250	0.02%	0.002%
17	3.867	781	786	791	rBV	230	249	0.02%	0.002%
18	3.996	821	826	830	rBV2	216	315	0.02%	0.002%
19	4.063	843	847	851	rBV2	197	210	0.01%	0.002%
20	4.124	859	866	868	rBV2	234	314	0.02%	0.002%
21	4.552	994	999	1003	rBV2	346	463	0.03%	0.004%
22	4.620	1007	1020	1049	rBV	167195	424257	26.25%	3.351%
23	4.796	1072	1075	1076	rBV2	575	314	0.02%	0.002%
24	4.848	1088	1091	1095	rVB2	413	322	0.02%	0.003%
25	4.874	1096	1099	1103	rBV3	426	271	0.02%	0.002%
26	5.063	1141	1158	1182	rVV	290356	631048	39.04%	4.984%
27	5.285	1221	1227	1228	rBV2	402	414	0.03%	0.003%
28	5.333	1234	1242	1244	rBV2	1173	1556	0.10%	0.012%
29	5.459	1279	1281	1287	rVB2	235	153	0.01%	0.001%
30	5.639	1334	1337	1342	rBV2	206	190	0.01%	0.002%
31	5.726	1342	1364	1399	rBV2	600919	1616326	100.00%	12.767%
32	5.919	1417	1424	1430	rVV6	1313	1851	0.11%	0.015%
33	5.960	1434	1437	1450	rVB5	1190	1867	0.12%	0.015%
34	6.034	1458	1460	1467	rVB3	512	501	0.03%	0.004%
35	6.111	1482	1484	1487	rBV2	331	239	0.01%	0.002%
36	6.250	1512	1527	1557	rBV	387592	745108	46.10%	5.885%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
 Title : VOC Analysis

37	6.526	1605	1613	1624	rBV5	2211	4032	0.25%	0.032%
38	6.591	1627	1633	1639	rBV4	622	698	0.04%	0.006%
39	6.690	1649	1664	1684	rBV	372990	721564	44.64%	5.699%
40	6.857	1712	1716	1718	rBV2	199	172	0.01%	0.001%
41	6.931	1729	1739	1743	rBV4	1450	2505	0.15%	0.020%
42	7.041	1761	1773	1801	rVV	73335	135282	8.37%	1.069%
43	7.304	1850	1855	1859	rBV2	311	324	0.02%	0.003%
44	7.565	1923	1936	1956	rBV	197534	344661	21.32%	2.722%
45	7.690	1970	1975	1977	rBV3	612	578	0.04%	0.005%
46	7.742	1981	1991	1999	rBV2	15066	24700	1.53%	0.195%
47	7.899	2026	2040	2055	rBV	748779	1273339	78.78%	10.058%
48	8.053	2086	2088	2092	rVB	477	307	0.02%	0.002%
49	8.179	2115	2127	2145	rBV	138402	235930	14.60%	1.864%
50	8.285	2158	2160	2163	rBV3	536	360	0.02%	0.003%
51	8.324	2169	2172	2175	rBV3	371	224	0.01%	0.002%
52	8.423	2199	2203	2207	rBV3	229	195	0.01%	0.002%
53	8.468	2207	2217	2227	rVB2	4429	7332	0.45%	0.058%
54	8.574	2238	2250	2257	rBV4	7382	12222	0.76%	0.097%
55	8.635	2257	2269	2289	rVV	534416	996665	61.66%	7.872%
56	8.729	2290	2298	2316	rVB	123977	206830	12.80%	1.634%
57	8.838	2324	2332	2346	rVB2	6526	11458	0.71%	0.091%
58	9.082	2405	2408	2411	rVB2	278	192	0.01%	0.002%
59	9.108	2411	2416	2423	rVB	412	471	0.03%	0.004%
60	9.163	2428	2433	2438	rVB3	349	321	0.02%	0.003%
61	9.211	2438	2448	2462	rBV	71063	113840	7.04%	0.899%
62	9.330	2482	2485	2488	rBV2	282	159	0.01%	0.001%
63	9.365	2492	2496	2497	rBV2	387	221	0.01%	0.002%
64	9.417	2499	2512	2532	rBV	602749	983030	60.82%	7.765%
65	9.642	2579	2582	2586	rBV2	378	327	0.02%	0.003%
66	9.700	2592	2600	2604	rVB3	820	1078	0.07%	0.009%
67	9.751	2613	2616	2618	rBV	332	254	0.02%	0.002%
68	9.893	2656	2660	2662	rBV	192	141	0.01%	0.001%
69	9.960	2678	2681	2684	rBV2	357	273	0.02%	0.002%
70	10.073	2712	2716	2717	rBV	732	455	0.03%	0.004%
71	10.195	2751	2754	2756	rBV2	213	165	0.01%	0.001%
72	10.221	2760	2762	2765	rBV2	186	148	0.01%	0.001%
73	10.272	2775	2778	2781	rBV2	189	185	0.01%	0.001%
74	10.407	2816	2820	2823	rBV2	187	146	0.01%	0.001%
75	10.442	2827	2831	2833	rBV	291	218	0.01%	0.002%
76	10.539	2855	2861	2864	rBV2	306	322	0.02%	0.003%

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 Title : VOC Analysis

77	10.597	2876	2879	2882	rBV2	286	222	0.01%	0.002%
78	10.674	2896	2903	2909	rVB2	2170	3047	0.19%	0.024%
79	10.758	2916	2929	2947	rVV	627638	1011597	62.59%	7.990%
80	10.864	2958	2962	2963	rBV	509	339	0.02%	0.003%
81	10.999	2999	3004	3008	rBV3	459	466	0.03%	0.004%
82	11.121	3035	3042	3045	rBV2	759	660	0.04%	0.005%
83	11.195	3063	3065	3069	rBV2	308	228	0.01%	0.002%
84	11.346	3108	3112	3119	rBV2	345	323	0.02%	0.003%
85	11.413	3128	3133	3136	rBV4	738	598	0.04%	0.005%
86	11.462	3140	3148	3152	rBV4	1432	2016	0.12%	0.016%
87	11.696	3217	3221	3225	rBV3	806	870	0.05%	0.007%
88	11.716	3225	3227	3230	rVB	241	134	0.01%	0.001%
89	11.812	3244	3257	3278	rBV	569006	900589	55.72%	7.113%
90	11.970	3303	3306	3314	rVB4	1651	1768	0.11%	0.014%
91	12.005	3315	3317	3322	rVV3	306	240	0.01%	0.002%
92	12.195	3363	3376	3395	rBV	702393	1139051	70.47%	8.997%
93	12.323	3414	3416	3417	rBV2	472	218	0.01%	0.002%
94	12.487	3464	3467	3468	rBV	322	196	0.01%	0.002%
95	12.539	3480	3483	3484	rBV	268	157	0.01%	0.001%
96	12.600	3499	3502	3505	rVB2	484	305	0.02%	0.002%
97	12.635	3511	3513	3516	rBV3	455	360	0.02%	0.003%
98	12.764	3550	3553	3563	rVB	807	1042	0.06%	0.008%
99	12.954	3610	3612	3615	rBV2	269	225	0.01%	0.002%
100	13.098	3651	3657	3662	rBV3	439	722	0.04%	0.006%

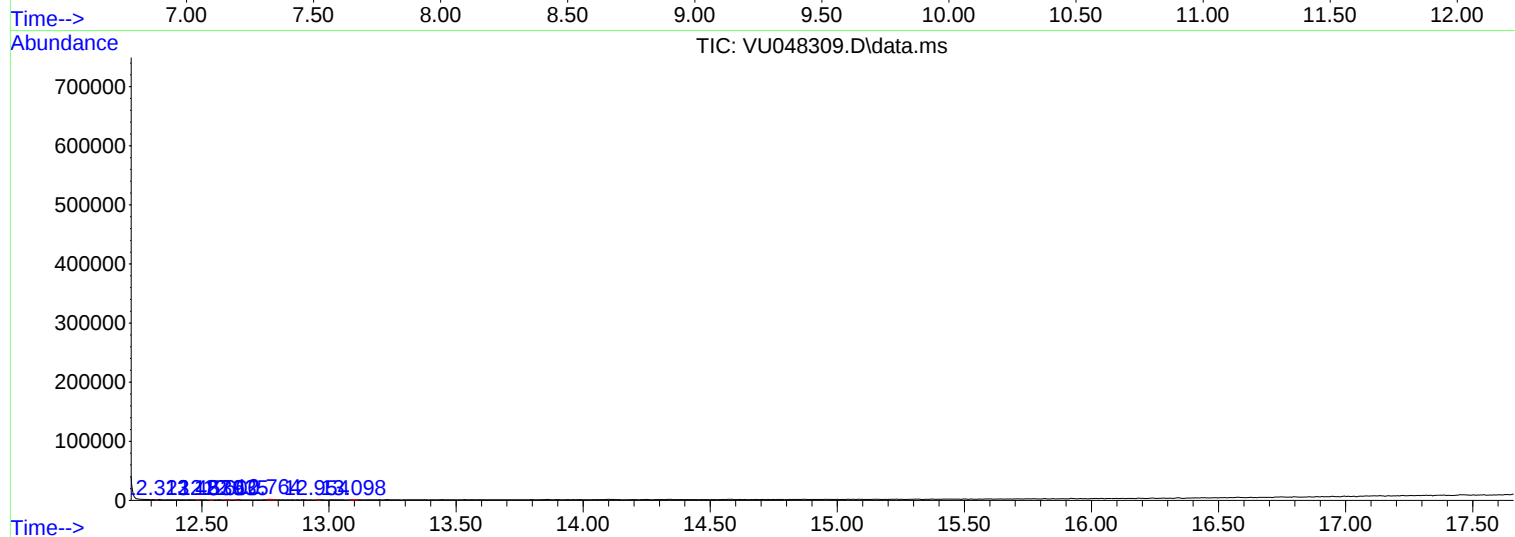
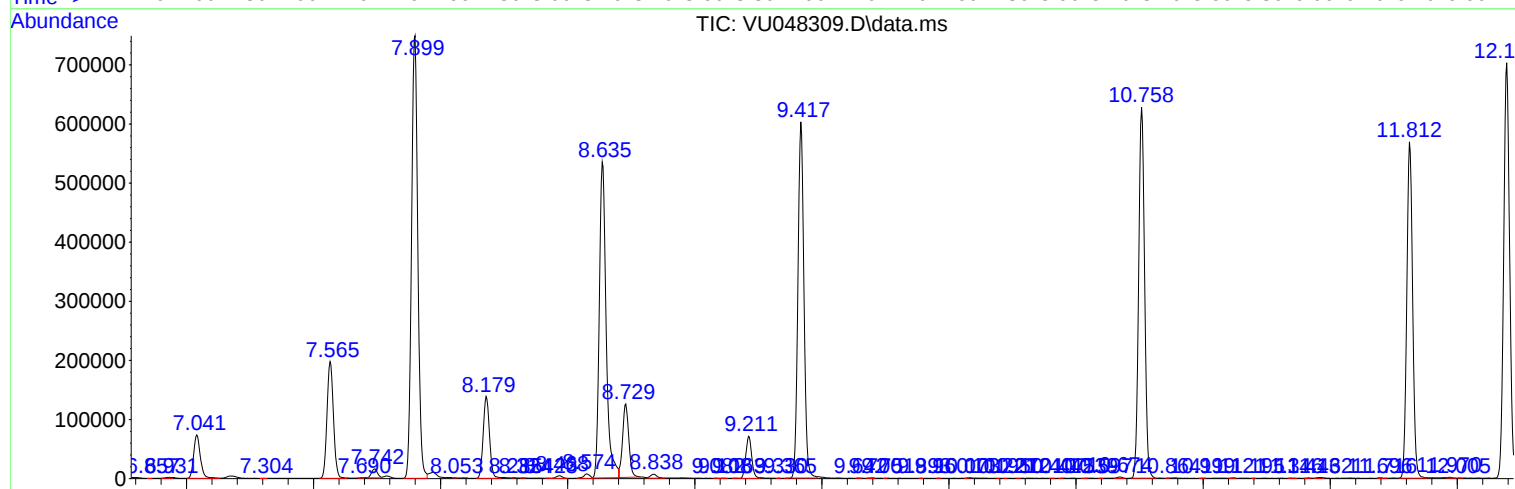
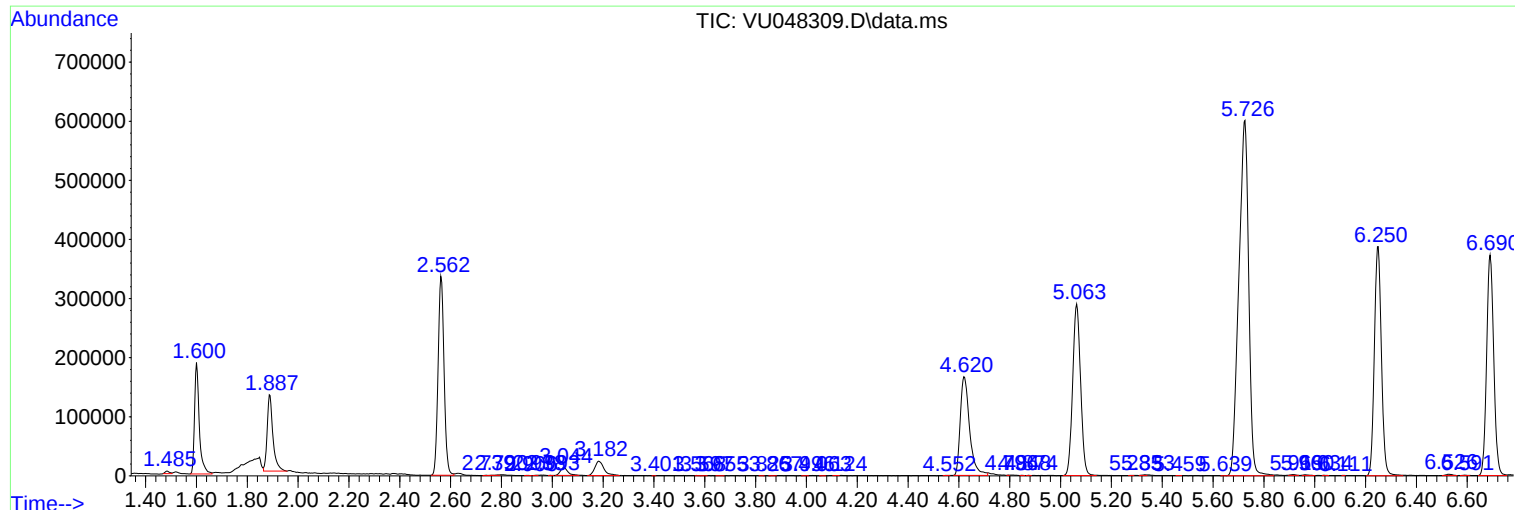
Sum of corrected areas: 12660558

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ClientSampleId :
EXER8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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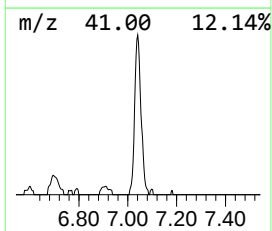
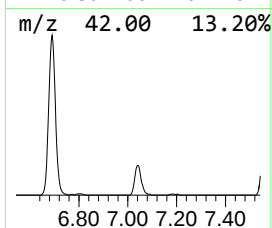
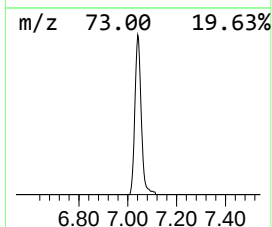
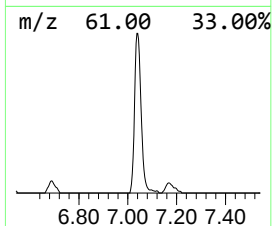
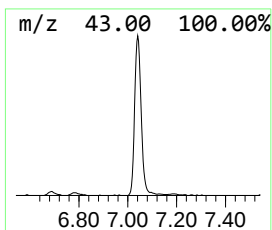
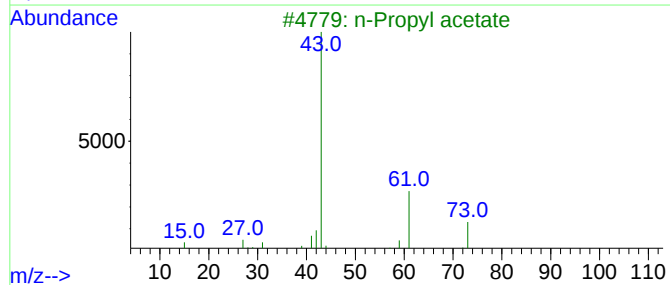
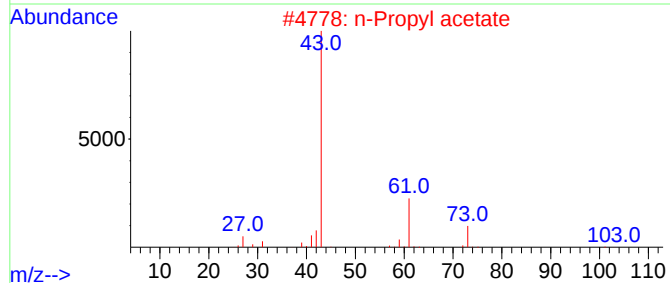
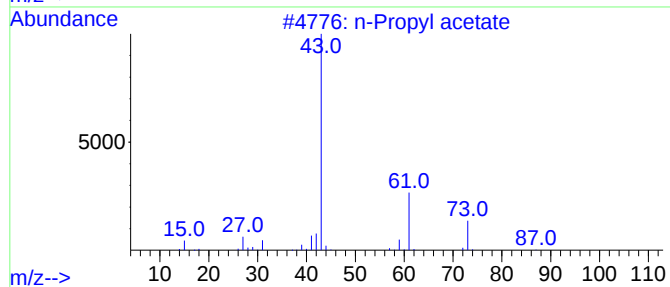
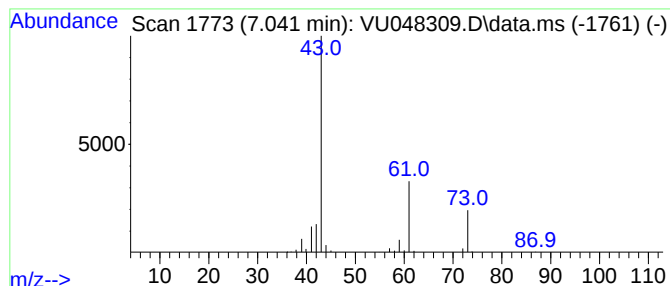
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	9.08 ug/L	135282	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	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	56



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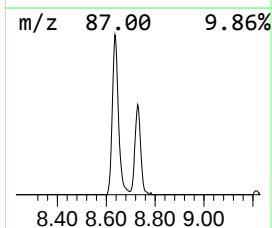
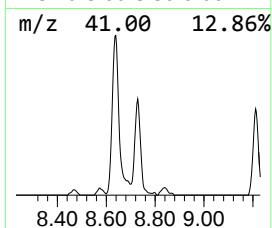
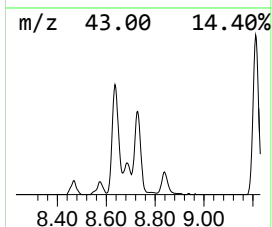
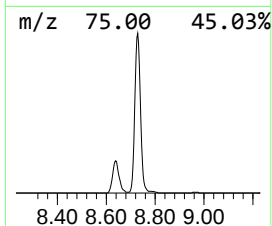
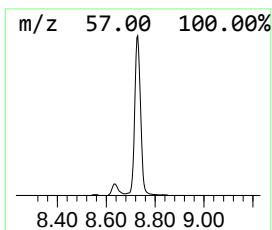
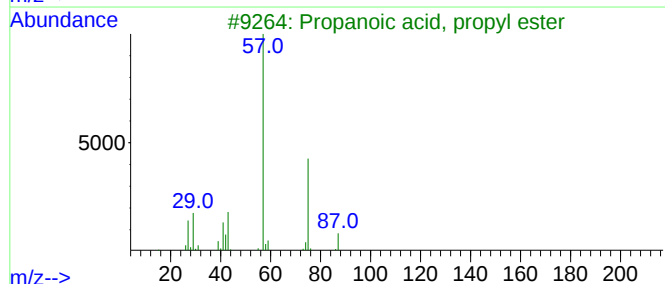
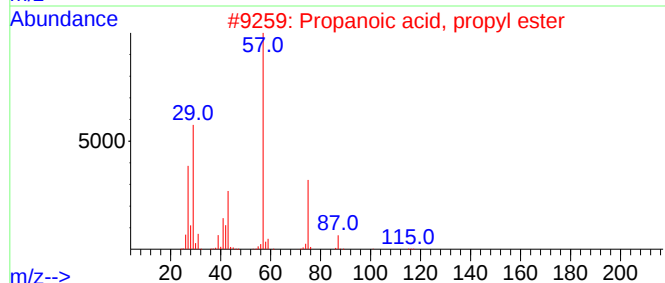
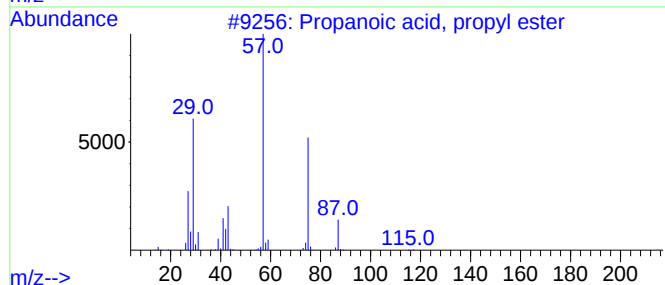
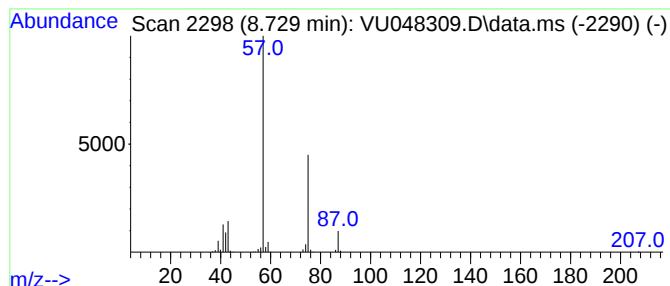
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	10.52 ug/L	206830	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	83
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64



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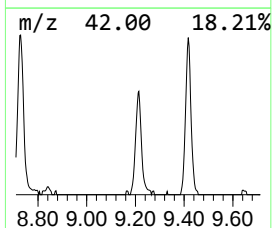
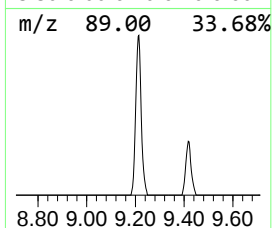
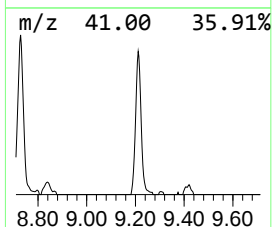
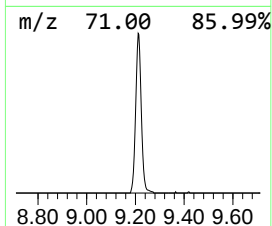
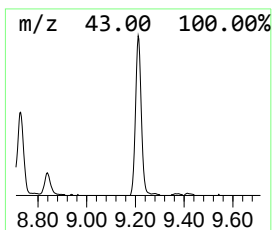
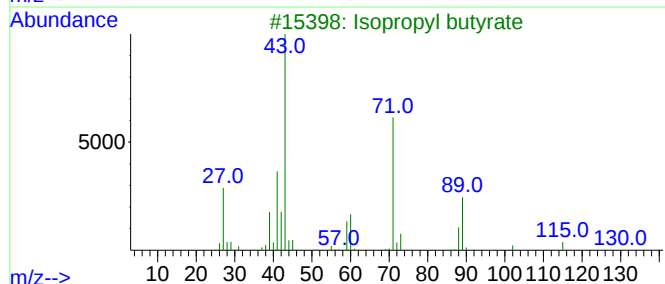
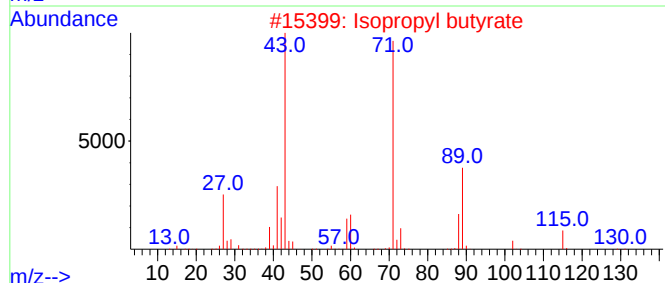
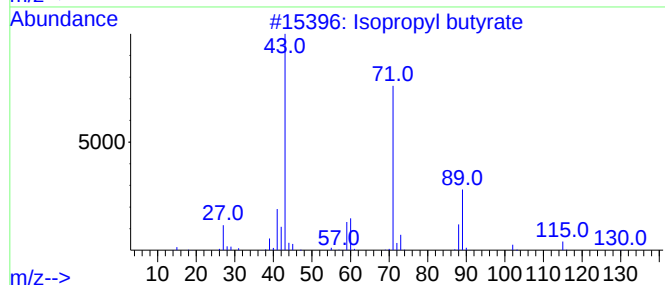
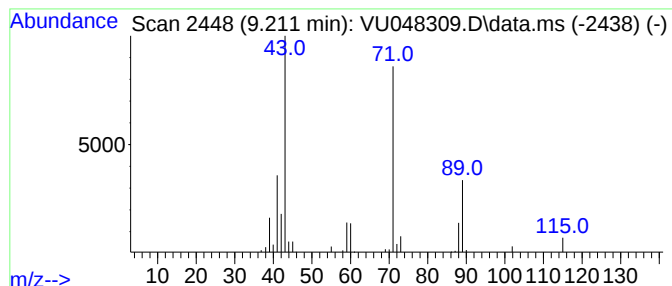
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	5.79 ug/L	113840	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			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042722\
Data File : VU048309.D
Acq On : 27 Apr 2022 13:08
Operator : SY/MD
Sample : N2542-02 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXER8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.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	9.1	ug/L	135282	1	6.250	745108	50.0
Propanoic acid,...	8.729	10.5	ug/L	206830	2	9.417	983030	50.0
Isopropyl butyrate	9.211	5.8	ug/L	113840	2	9.417	983030	50.0