

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042722\
 Data File : VU048308.D
 Acq On : 27 Apr 2022 12:44
 Operator : SY/MD
 Sample : N2542-01 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNS5

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: VU048308.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	39	45	51	rBV3	5239	7427	0.46%	0.058%
2	1.601	73	81	101	rBV	187279	243535	15.03%	1.898%
3	1.884	163	169	192	rVB	131561	206309	12.73%	1.608%
4	2.562	366	380	396	rBV	334330	552787	34.12%	4.308%
5	2.758	438	441	443	rBV2	500	322	0.02%	0.003%
6	2.790	447	451	452	rVV2	541	385	0.02%	0.003%
7	2.951	498	501	503	rBV2	497	306	0.02%	0.002%
8	3.044	520	530	546	rBV	10323	21969	1.36%	0.171%
9	3.183	558	573	590	rBV	27370	66231	4.09%	0.516%
10	3.379	630	634	636	rBV3	231	183	0.01%	0.001%
11	3.456	654	658	663	rVV2	320	268	0.02%	0.002%
12	3.594	696	701	704	rBV	254	249	0.02%	0.002%
13	3.671	719	725	728	rBV2	182	225	0.01%	0.002%
14	3.703	732	735	739	rBV	214	243	0.01%	0.002%
15	3.803	764	766	769	rVB	376	201	0.01%	0.002%
16	3.832	769	775	777	rBV2	318	371	0.02%	0.003%
17	3.977	818	820	827	rVB2	297	324	0.02%	0.003%
18	4.118	861	864	867	rVV3	440	309	0.02%	0.002%
19	4.183	880	884	888	rBV2	247	281	0.02%	0.002%
20	4.549	994	998	1003	rVV2	476	482	0.03%	0.004%
21	4.620	1007	1020	1071	rVV	163928	425898	26.28%	3.319%
22	4.858	1092	1094	1097	rVB	528	226	0.01%	0.002%
23	4.887	1101	1103	1109	rVB3	324	223	0.01%	0.002%
24	4.941	1116	1120	1124	rBV2	279	324	0.02%	0.003%
25	5.064	1140	1158	1178	rBV	288980	634192	39.14%	4.942%
26	5.189	1194	1197	1202	rVB2	330	245	0.02%	0.002%
27	5.295	1221	1230	1232	rBV3	501	703	0.04%	0.005%
28	5.330	1236	1241	1243	rBV3	948	880	0.05%	0.007%
29	5.723	1342	1363	1404	rBV2	605292	1620363	100.00%	12.627%
30	5.867	1404	1408	1411	rBV2	501	467	0.03%	0.004%
31	5.916	1418	1423	1432	rVB3	1453	2122	0.13%	0.017%
32	5.973	1432	1441	1450	rVB5	1232	2060	0.13%	0.016%
33	6.044	1458	1463	1469	rVB4	491	506	0.03%	0.004%
34	6.144	1491	1494	1498	rVB3	293	223	0.01%	0.002%
35	6.247	1512	1526	1547	rBV	396526	754757	46.58%	5.882%
36	6.491	1599	1602	1606	rBV2	295	259	0.02%	0.002%

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 Title : VOC Analysis

37	6.520	1606	1611	1612	rBV2	1588	1116	0.07%	0.009%
38	6.597	1628	1635	1636	rBV3	460	418	0.03%	0.003%
39	6.690	1649	1664	1685	rBV	377320	728703	44.97%	5.679%
40	6.787	1690	1694	1698	rVB4	691	581	0.04%	0.005%
41	6.928	1724	1738	1744	rBV4	1831	3682	0.23%	0.029%
42	7.041	1760	1773	1791	rBV	75422	137495	8.49%	1.071%
43	7.170	1803	1813	1816	rBV2	3982	5335	0.33%	0.042%
44	7.256	1835	1840	1845	rVB3	366	363	0.02%	0.003%
45	7.372	1869	1876	1879	rBV2	157	187	0.01%	0.001%
46	7.565	1922	1936	1957	rBV	199681	346992	21.41%	2.704%
47	7.678	1967	1971	1975	rBV4	883	1015	0.06%	0.008%
48	7.739	1980	1990	2000	rVV2	17081	29327	1.81%	0.229%
49	7.790	2000	2006	2015	rVV4	4408	7534	0.46%	0.059%
50	7.896	2025	2039	2055	rBV	748383	1282506	79.15%	9.994%
51	8.179	2115	2127	2143	rBV	143890	240674	14.85%	1.876%
52	8.411	2196	2199	2200	rBV	324	190	0.01%	0.001%
53	8.465	2207	2216	2225	rBV3	4183	6635	0.41%	0.052%
54	8.578	2237	2251	2258	rBV5	7752	13734	0.85%	0.107%
55	8.636	2258	2269	2289	rVV	534176	988475	61.00%	7.703%
56	8.729	2290	2298	2314	rVB	130390	218039	13.46%	1.699%
57	8.838	2324	2332	2347	rVB	7452	13234	0.82%	0.103%
58	8.899	2347	2351	2353	rBV3	585	378	0.02%	0.003%
59	8.993	2376	2380	2381	rBV2	290	234	0.01%	0.002%
60	9.131	2420	2423	2427	rBV	320	288	0.02%	0.002%
61	9.169	2430	2435	2437	rBV4	437	422	0.03%	0.003%
62	9.211	2437	2448	2464	rBV	74707	120060	7.41%	0.936%
63	9.417	2492	2512	2547	rBV	606859	1014798	62.63%	7.908%
64	9.562	2554	2557	2558	rBV	387	227	0.01%	0.002%
65	9.575	2558	2561	2566	rVB2	636	523	0.03%	0.004%
66	9.642	2578	2582	2585	rBV3	433	422	0.03%	0.003%
67	9.684	2592	2595	2597	rBV	605	490	0.03%	0.004%
68	9.870	2649	2653	2655	rVV2	283	228	0.01%	0.002%
69	9.960	2679	2681	2687	rVB2	291	256	0.02%	0.002%
70	10.031	2697	2703	2708	rBV2	425	541	0.03%	0.004%
71	10.079	2712	2718	2722	rBV4	1120	1406	0.09%	0.011%
72	10.321	2789	2793	2795	rBV2	471	347	0.02%	0.003%
73	10.481	2840	2843	2849	rVB2	375	425	0.03%	0.003%
74	10.668	2896	2901	2910	rVB3	2379	2953	0.18%	0.023%
75	10.758	2916	2929	2948	rBV	626570	1009778	62.32%	7.869%
76	10.867	2960	2963	2967	rBV2	497	446	0.03%	0.003%

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 Title : VOC Analysis

77	10.883	2967	2968	2970	rBV	410	208	0.01%	0.002%
78	10.996	2998	3003	3009	rVB2	245	244	0.02%	0.002%
79	11.092	3030	3033	3036	rBV	525	326	0.02%	0.003%
80	11.112	3036	3039	3046	rBV4	789	881	0.05%	0.007%
81	11.276	3085	3090	3093	rBV	449	512	0.03%	0.004%
82	11.414	3130	3133	3135	rBV2	483	310	0.02%	0.002%
83	11.456	3139	3146	3150	rBV2	1279	1784	0.11%	0.014%
84	11.694	3215	3220	3226	rBV3	768	950	0.06%	0.007%
85	11.719	3226	3228	3233	rVB2	381	250	0.02%	0.002%
86	11.748	3233	3237	3244	rBV3	812	834	0.05%	0.006%
87	11.812	3244	3257	3280	rBV	584707	927876	57.26%	7.231%
88	11.976	3302	3308	3314	rVB5	1833	2240	0.14%	0.017%
89	12.195	3359	3376	3399	rBV	712554	1164257	71.85%	9.073%
90	12.324	3414	3416	3421	rVB5	689	346	0.02%	0.003%
91	12.433	3445	3450	3451	rBV2	288	266	0.02%	0.002%
92	12.565	3488	3491	3495	rBV2	315	266	0.02%	0.002%
93	12.771	3550	3555	3563	rVB3	1188	1702	0.11%	0.013%
94	13.031	3634	3636	3644	rVB2	502	472	0.03%	0.004%
95	13.066	3644	3647	3651	rVB2	324	229	0.01%	0.002%
96	13.095	3653	3656	3659	rBV	331	309	0.02%	0.002%
97	13.147	3668	3672	3675	rBV2	475	436	0.03%	0.003%
98	15.073	4269	4271	4274	rBV2	492	334	0.02%	0.003%
99	15.655	4450	4452	4455	rBV2	654	327	0.02%	0.003%
100	15.674	4455	4458	4461	rBV3	875	607	0.04%	0.005%

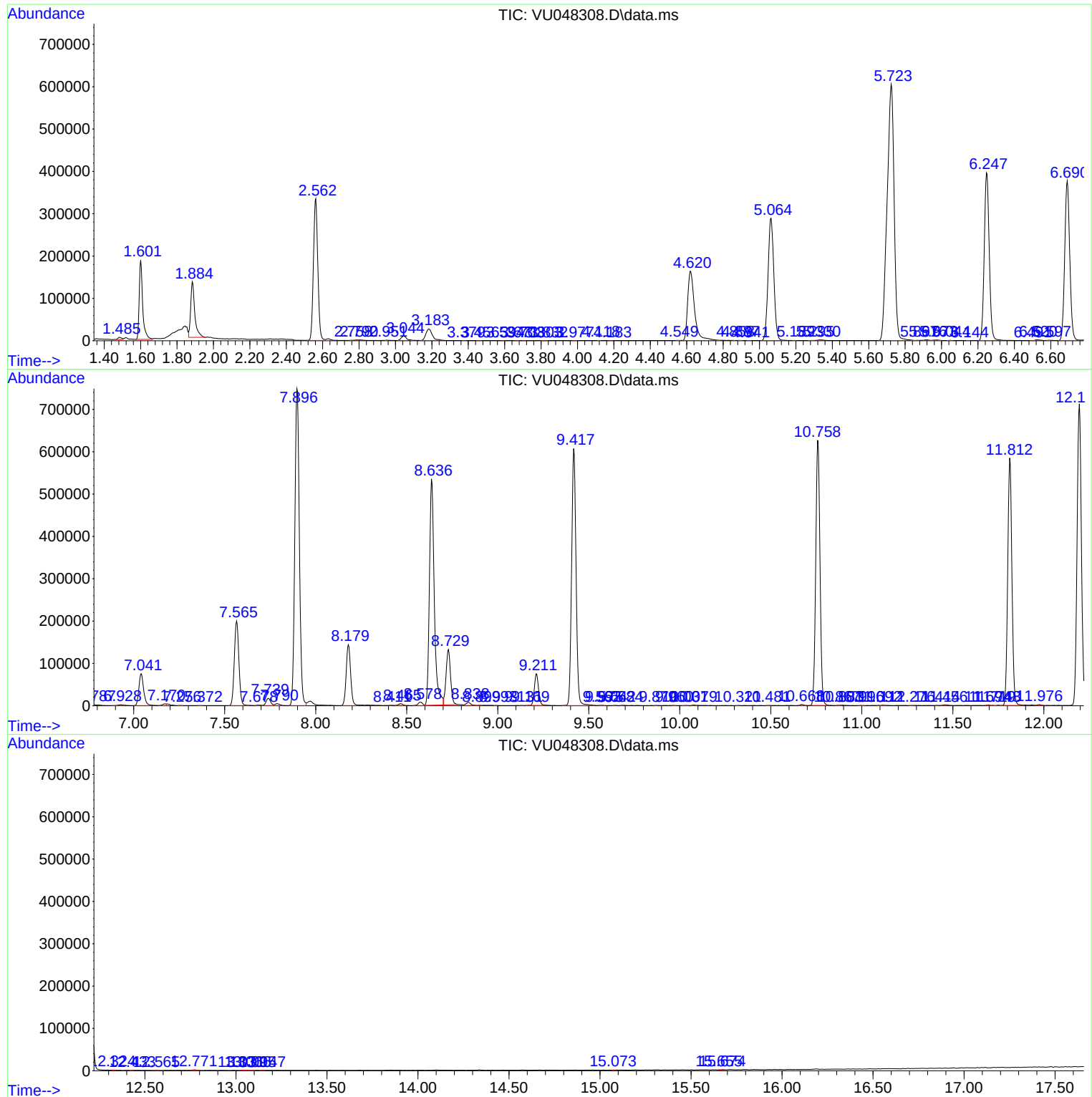
Sum of corrected areas: 12832278

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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



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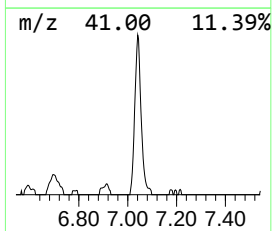
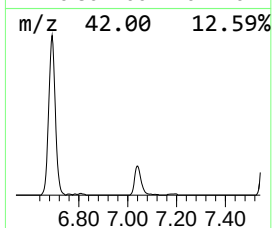
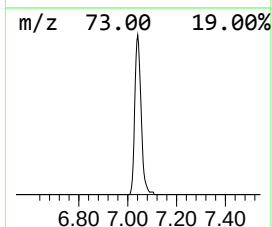
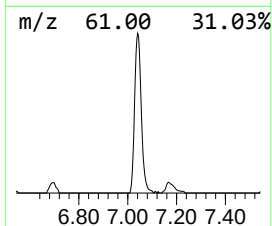
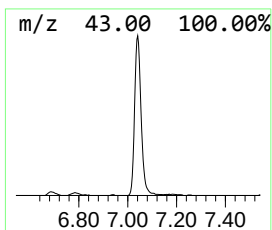
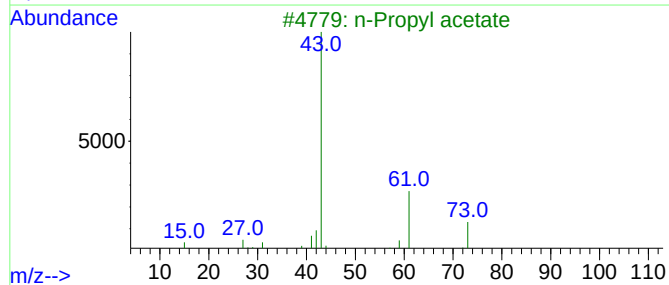
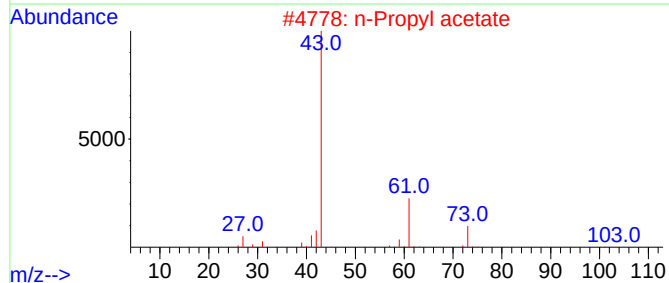
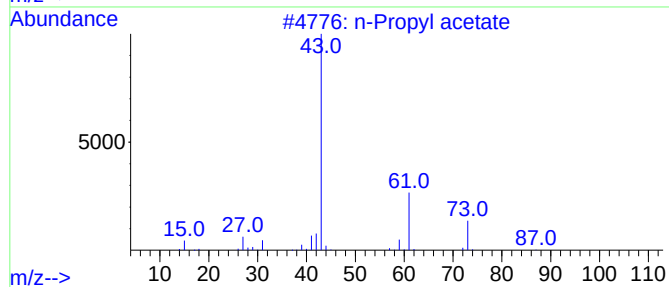
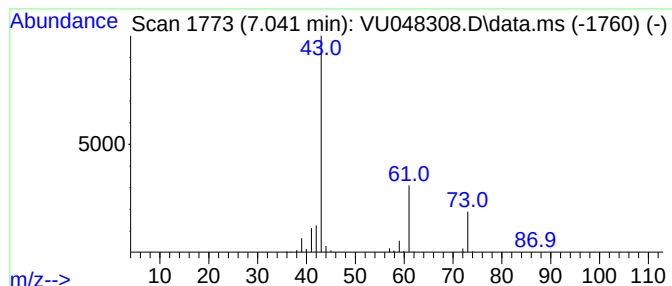
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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	9.11 ug/L	137495	1,4-Difluorobenzene	6.247

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	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	50



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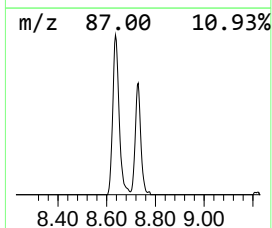
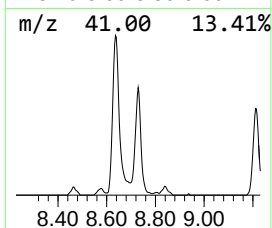
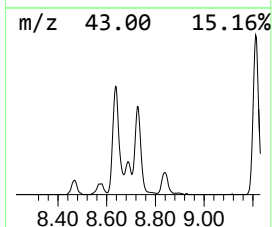
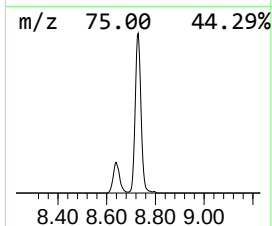
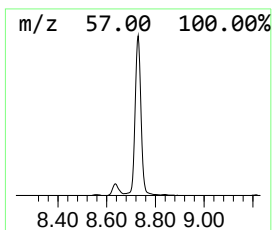
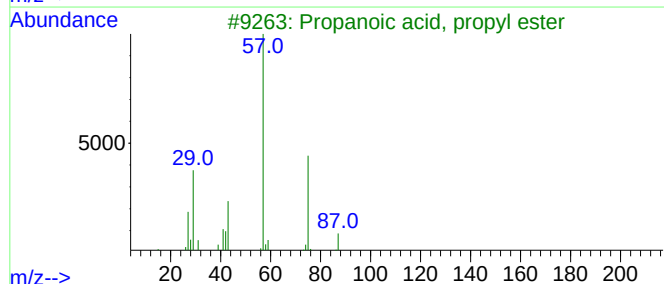
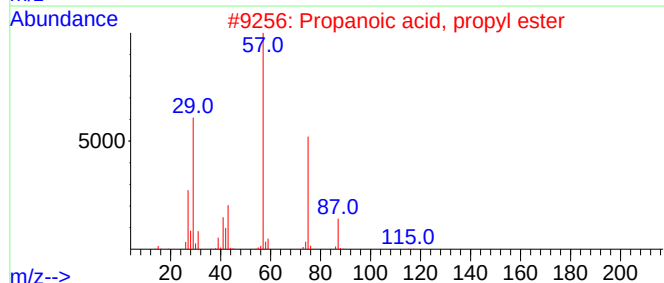
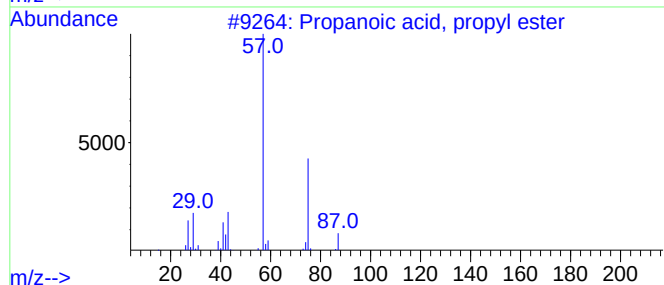
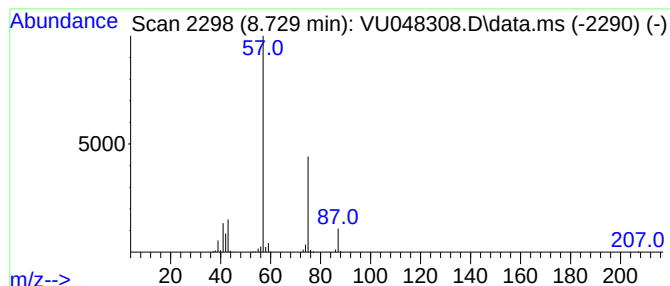
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	10.74 ug/L	218039	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	78
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	33



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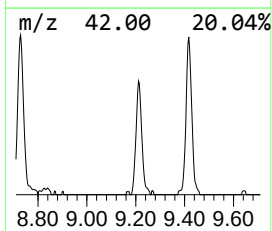
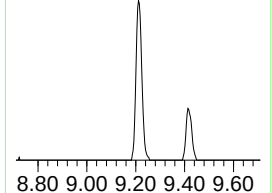
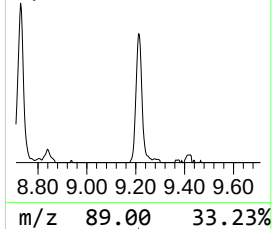
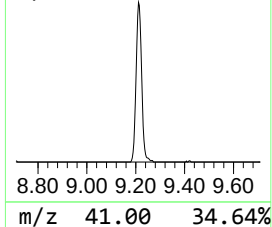
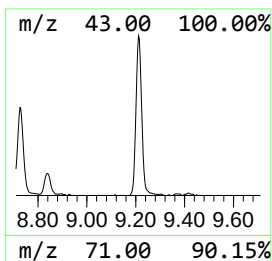
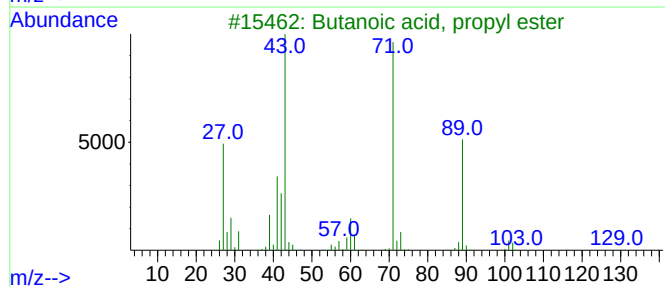
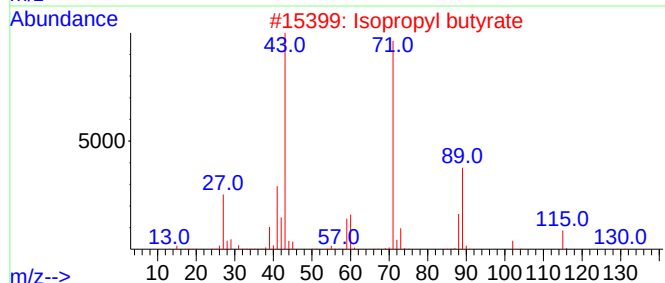
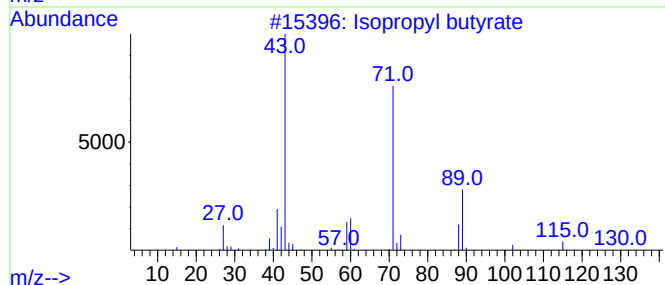
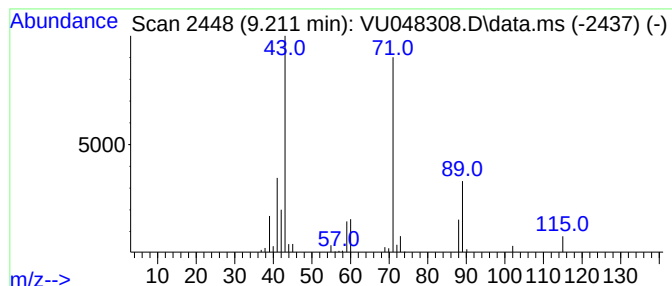
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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	5.92 ug/L	120060	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			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78
5			Isopropyl butyrate	130	C7H14O2	000638-11-9	78



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Operator : SY/MD
Sample : N2542-01 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNS5

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	137495	1	6.247	754757	50.0
Propanoic acid,...	8.729	10.7	ug/L	218039	2	9.417	1014800	50.0
Isopropyl butyrate	9.211	5.9	ug/L	120060	2	9.417	1014800	50.0