

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
 Data File : VU042279.D
 Acq On : 05 Feb 2021 13:42
 Operator : SY/MD
 Sample : PB134469TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB001

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\SFAMULM020521WMA.M

Title : VOC Analysis

Signal : TIC: VU042279.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	74	81	99	rVB	93210	113699	13.84%	1.636%
2	1.912	172	178	195	rVB	61382	77941	9.49%	1.121%
3	2.568	369	382	403	rBV	184134	314014	38.22%	4.517%
4	2.758	437	441	443	rVB	266	193	0.02%	0.003%
5	2.954	498	502	504	rBV	175	163	0.02%	0.002%
6	3.051	523	532	543	rVB2	2166	3599	0.44%	0.052%
7	3.192	566	576	589	rBV2	2364	5210	0.63%	0.075%
8	3.411	642	644	646	rBV	175	70	0.01%	0.001%
9	3.649	717	718	722	rVB	125	70	0.01%	0.001%
10	3.674	723	726	728	rBV	106	68	0.01%	0.001%
11	3.764	746	754	756	rBV	94	104	0.01%	0.001%
12	3.845	770	779	783	rVV2	488	805	0.10%	0.012%
13	3.861	783	784	791	rVB	301	117	0.01%	0.002%
14	3.899	791	796	802	rBV2	216	197	0.02%	0.003%
15	3.967	814	817	821	rVV	171	138	0.02%	0.002%
16	3.993	821	825	828	rVV	104	71	0.01%	0.001%
17	4.025	833	835	842	rVB	200	118	0.01%	0.002%
18	4.305	918	922	925	rBV	131	93	0.01%	0.001%
19	4.395	947	950	955	rVB	139	98	0.01%	0.001%
20	4.427	955	960	966	rBV	84	102	0.01%	0.001%
21	4.485	977	978	981	rVB	159	78	0.01%	0.001%
22	4.517	985	988	991	rBV2	207	140	0.02%	0.002%
23	4.645	1012	1028	1059	rBV	73925	232513	28.30%	3.345%
24	4.922	1111	1114	1123	rBV2	194	193	0.02%	0.003%
25	4.989	1133	1135	1141	rBV	97	74	0.01%	0.001%
26	5.073	1145	1161	1186	rVV	150005	328918	40.04%	4.731%
27	5.288	1224	1228	1231	rBV3	525	493	0.06%	0.007%
28	5.382	1252	1257	1261	rVB2	530	397	0.05%	0.006%
29	5.494	1290	1292	1296	rBV	170	72	0.01%	0.001%
30	5.539	1302	1306	1308	rBV	128	72	0.01%	0.001%
31	5.578	1314	1318	1319	rBV	203	144	0.02%	0.002%
32	5.607	1324	1327	1332	rBV	90	70	0.01%	0.001%
33	5.629	1332	1334	1338	rVB	218	106	0.01%	0.002%
34	5.732	1344	1366	1388	rBV2	307800	821537	100.00%	11.817%
35	5.928	1419	1427	1440	rVB3	1108	2270	0.28%	0.033%
36	5.980	1440	1443	1449	rBV3	309	290	0.04%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
 Title : VOC Analysis

37	6.021	1453	1456	1458	rBV	143	84	0.01%	0.001%
38	6.050	1462	1465	1468	rBV3	218	171	0.02%	0.002%
39	6.124	1484	1488	1492	rBV3	256	171	0.02%	0.002%
40	6.160	1494	1499	1501	rBV4	384	311	0.04%	0.004%
41	6.256	1515	1529	1562	rBV	244561	464947	56.59%	6.688%
42	6.465	1592	1594	1596	rVB	174	88	0.01%	0.001%
43	6.484	1596	1600	1602	rBV	183	84	0.01%	0.001%
44	6.501	1602	1605	1609	rBV2	220	136	0.02%	0.002%
45	6.539	1609	1617	1621	rVB4	1119	1545	0.19%	0.022%
46	6.594	1631	1634	1636	rBV2	396	236	0.03%	0.003%
47	6.700	1653	1667	1688	rBV	195548	375079	45.66%	5.395%
48	6.771	1688	1689	1692	rBV	480	334	0.04%	0.005%
49	6.935	1733	1740	1741	rBV2	980	878	0.11%	0.013%
50	7.054	1762	1777	1796	rBV	82367	166358	20.25%	2.393%
51	7.205	1817	1824	1828	rBV6	765	981	0.12%	0.014%
52	7.253	1837	1839	1842	rVB	152	85	0.01%	0.001%
53	7.295	1850	1852	1856	rVB	168	78	0.01%	0.001%
54	7.382	1874	1879	1884	rBV	94	108	0.01%	0.002%
55	7.501	1914	1916	1918	rBV	147	79	0.01%	0.001%
56	7.574	1926	1939	1962	rBV	112952	202022	24.59%	2.906%
57	7.693	1974	1976	1982	rVB3	308	187	0.02%	0.003%
58	7.755	1983	1995	2006	rBV	12741	23237	2.83%	0.334%
59	7.906	2028	2042	2061	rBV	375330	644027	78.39%	9.264%
60	8.073	2091	2094	2097	rVB	177	97	0.01%	0.001%
61	8.099	2097	2102	2103	rBV	296	186	0.02%	0.003%
62	8.189	2117	2130	2152	rVB	81080	141570	17.23%	2.036%
63	8.269	2153	2155	2162	rVB2	356	334	0.04%	0.005%
64	8.478	2211	2220	2229	rBV4	4095	6666	0.81%	0.096%
65	8.539	2236	2239	2241	rBV	133	82	0.01%	0.001%
66	8.591	2244	2255	2262	rVV4	9271	15913	1.94%	0.229%
67	8.655	2262	2275	2291	rVV	268988	506287	61.63%	7.283%
68	8.742	2292	2302	2321	rVB	141754	240828	29.31%	3.464%
69	8.851	2326	2336	2347	rVB2	14877	25553	3.11%	0.368%
70	8.925	2354	2359	2361	rBV3	722	602	0.07%	0.009%
71	9.012	2383	2386	2388	rBV	203	122	0.01%	0.002%
72	9.224	2440	2452	2467	rBV	91384	147877	18.00%	2.127%
73	9.372	2493	2498	2502	rBV2	320	404	0.05%	0.006%
74	9.426	2502	2515	2535	rVV	336884	560262	68.20%	8.059%
75	9.581	2558	2563	2565	rBV	404	323	0.04%	0.005%
76	9.754	2614	2617	2619	rBV	166	76	0.01%	0.001%

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Integrator: RTE

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Peak Location: TOP

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77	9.912	2662	2666	2669	rBV	107	106	0.01%	0.002%
78	10.086	2712	2720	2728	rBV3	3380	4801	0.58%	0.069%
79	10.439	2826	2830	2833	rBV	116	105	0.01%	0.002%
80	10.770	2920	2933	2948	rBV	265546	425884	51.84%	6.126%
81	10.889	2966	2970	2973	rBV	158	108	0.01%	0.002%
82	11.098	3028	3035	3041	rBV3	529	903	0.11%	0.013%
83	11.124	3041	3043	3046	rVB	229	125	0.02%	0.002%
84	11.658	3206	3209	3210	rBV	135	82	0.01%	0.001%
85	11.751	3235	3238	3239	rBV	394	241	0.03%	0.003%
86	11.822	3248	3260	3277	rVB	337181	525179	63.93%	7.554%
87	12.205	3366	3379	3393	rVB	351035	555848	67.66%	7.996%
88	12.690	3527	3530	3532	rBV	152	96	0.01%	0.001%
89	12.780	3553	3558	3560	rBV	331	311	0.04%	0.004%
90	12.828	3570	3573	3575	rBV	252	156	0.02%	0.002%
91	13.098	3653	3657	3660	rBV2	285	240	0.03%	0.003%
92	13.510	3782	3785	3788	rVB2	213	126	0.02%	0.002%
93	13.822	3880	3882	3886	rBV	217	142	0.02%	0.002%
94	13.851	3886	3891	3898	rVV4	1140	1409	0.17%	0.020%
95	14.098	3961	3968	3973	rBV	1615	2309	0.28%	0.033%
96	14.430	4068	4071	4073	rBV2	273	183	0.02%	0.003%
97	14.597	4120	4123	4128	rBV2	394	292	0.04%	0.004%
98	14.687	4148	4151	4152	rBV2	251	111	0.01%	0.002%
99	14.700	4152	4155	4159	rVV2	327	271	0.03%	0.004%
100	14.799	4183	4186	4188	rBV	346	244	0.03%	0.004%

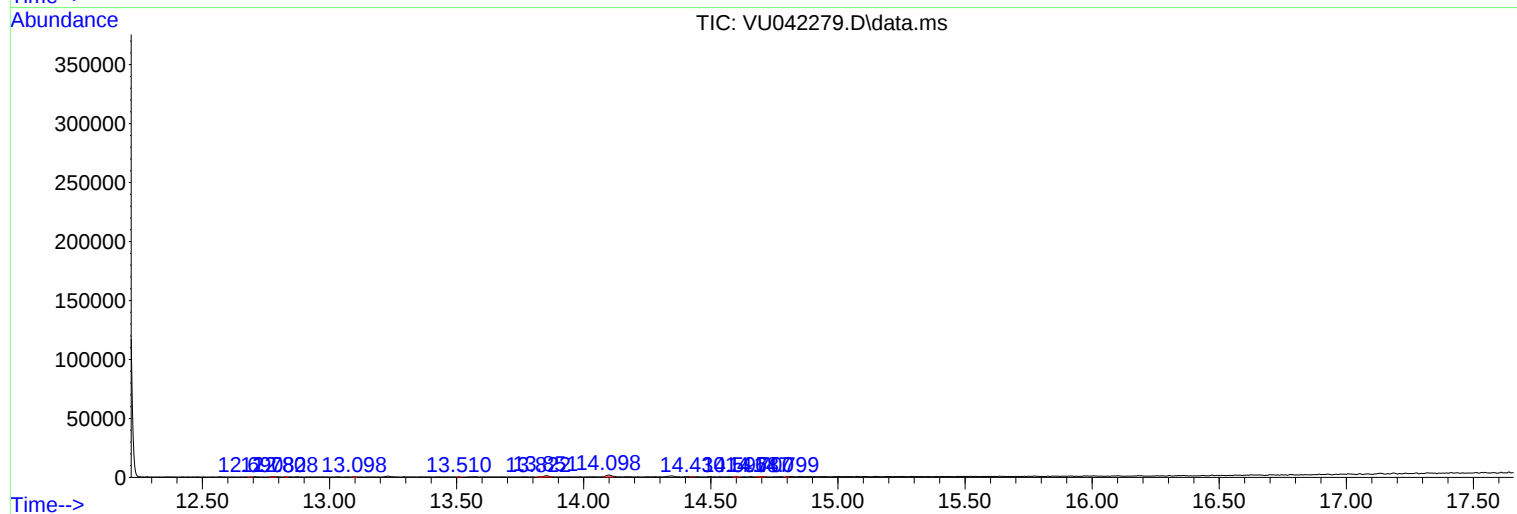
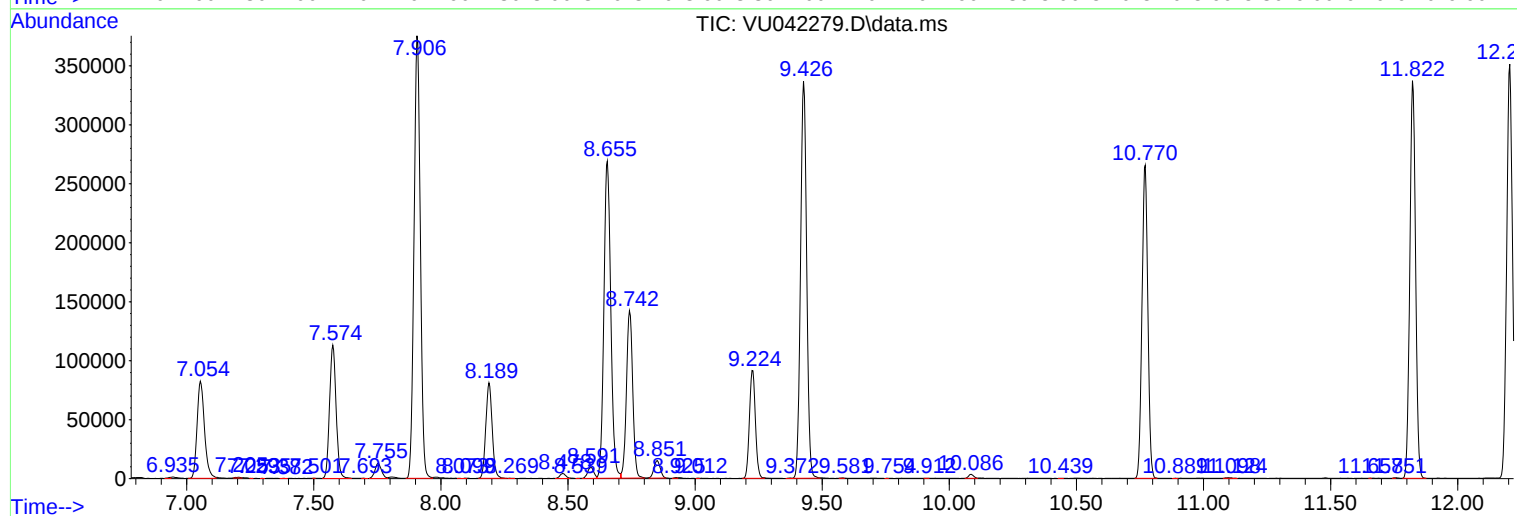
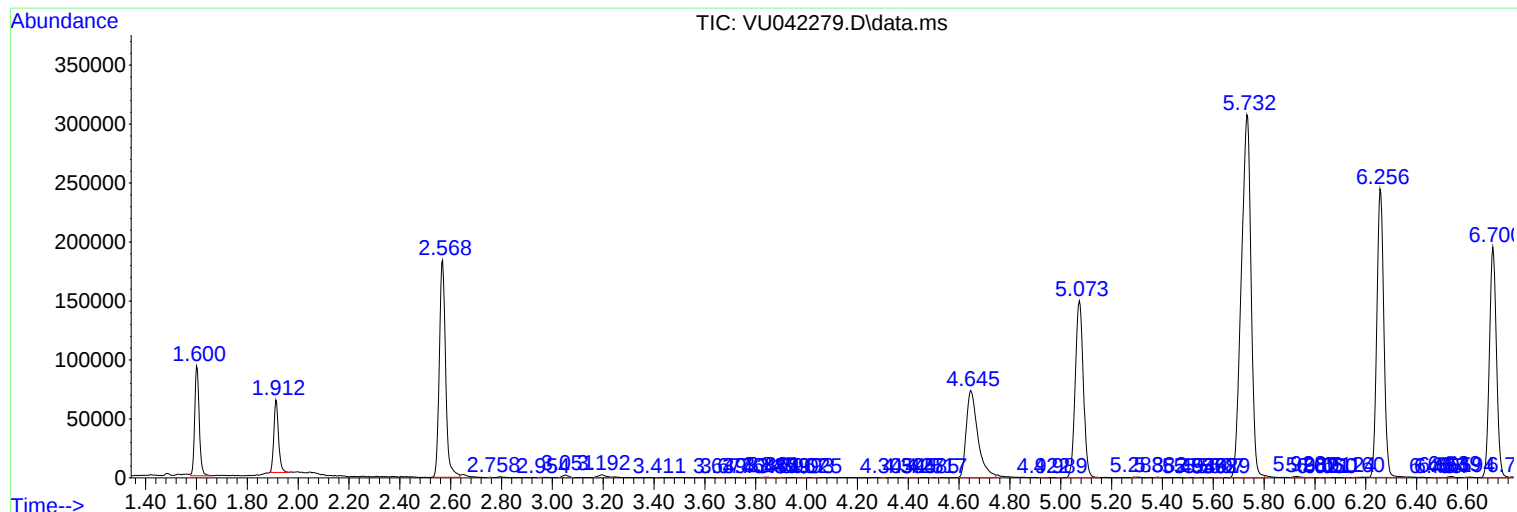
Sum of corrected areas: 6951917

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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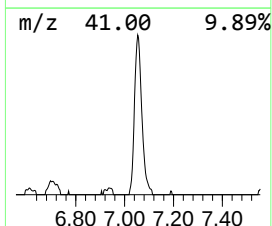
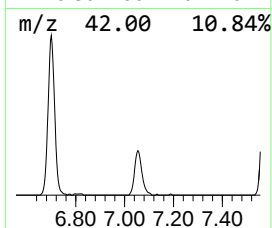
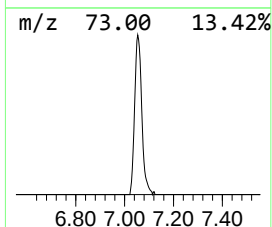
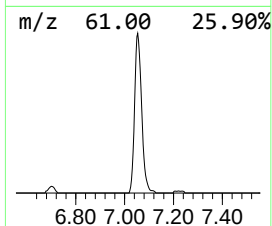
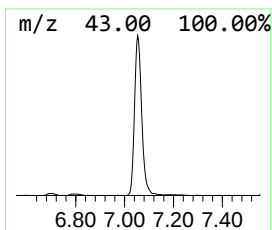
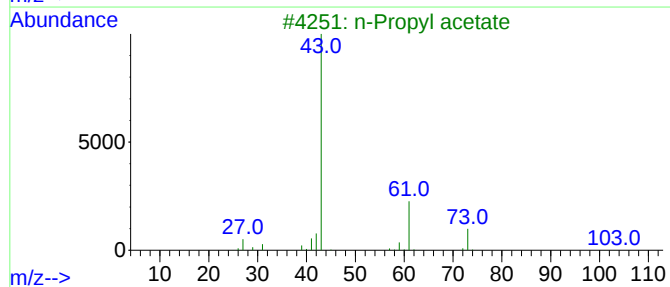
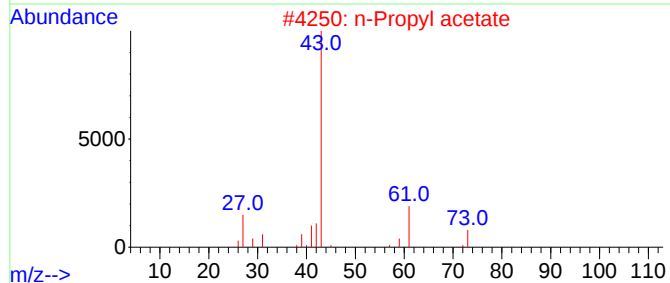
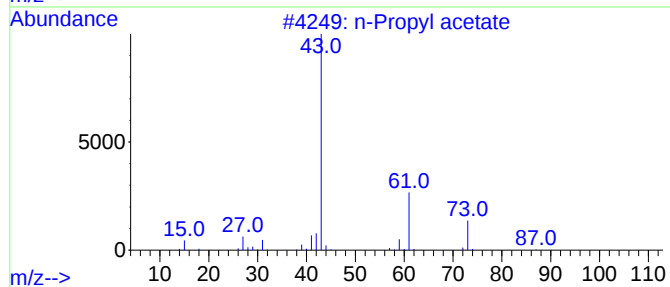
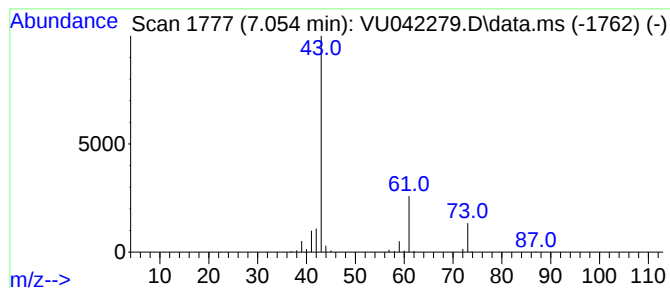
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.054	17.89 ug/L	166358	1,4-Difluorobenzene	6.256

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	74
4	Isopropyl acetate			102	C5H10O2	000108-21-4	36
5	Isopropyl acetate			102	C5H10O2	000108-21-4	9



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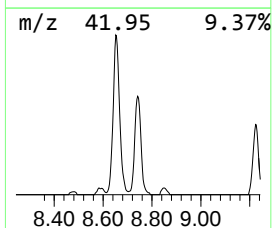
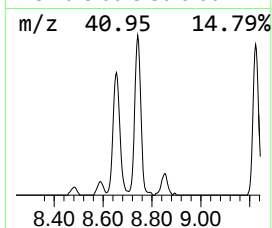
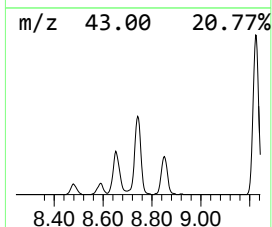
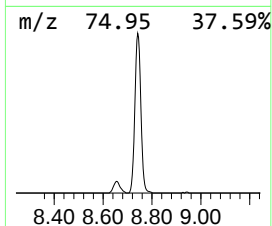
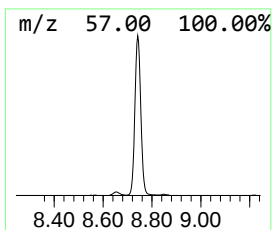
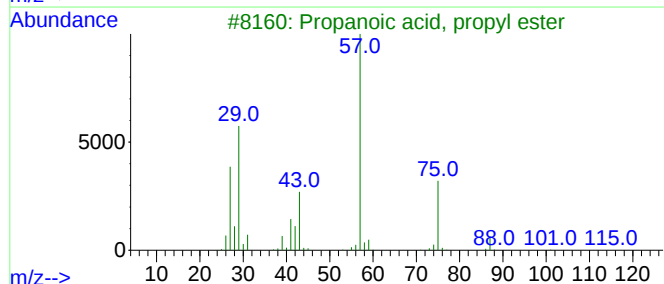
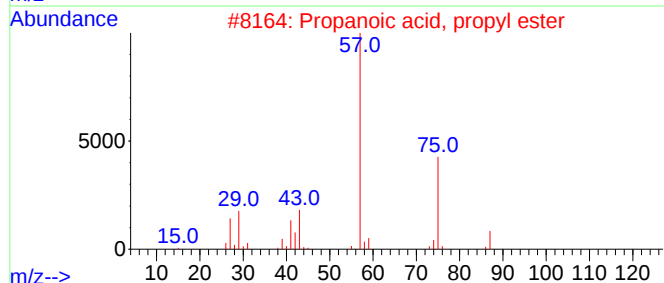
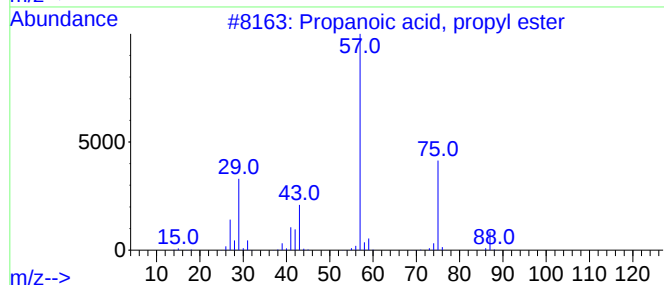
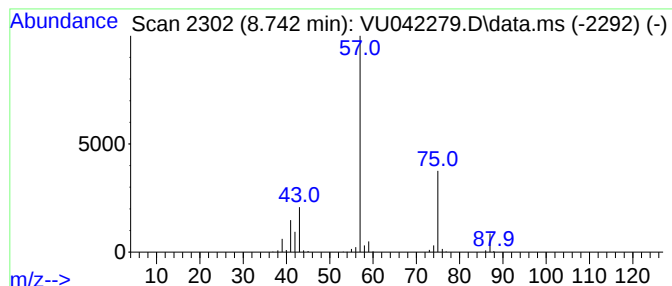
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.742	21.49 ug/L	240828	Chlorobenzene-d5	9.426

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	74
5			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	36



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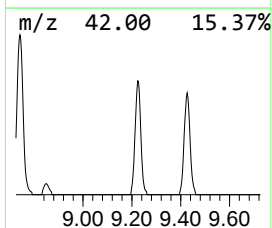
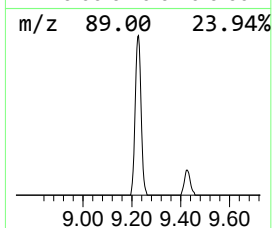
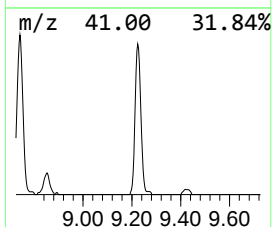
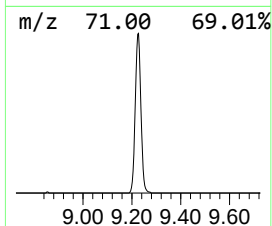
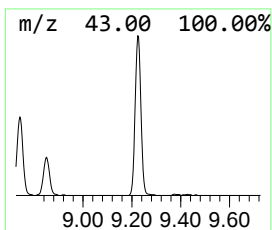
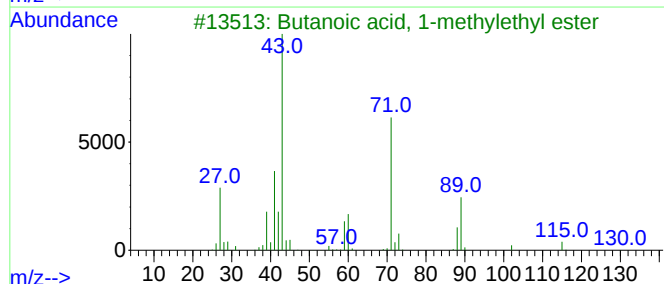
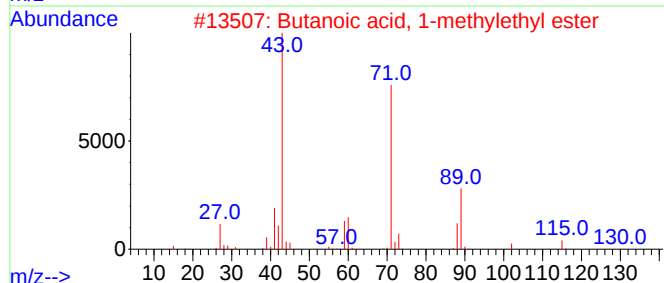
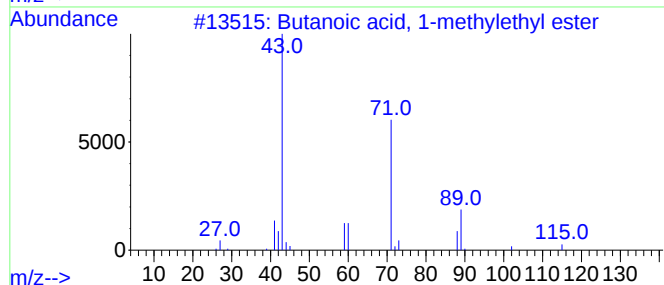
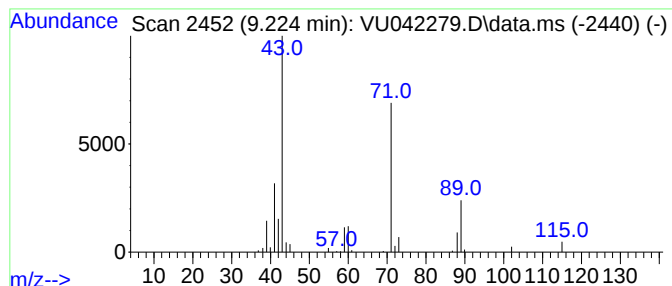
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butanoic acid, 1-methylethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.224	13.20 ug/L	147877	Chlorobenzene-d5	9.426

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
4			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	86
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042279.D
Acq On : 05 Feb 2021 13:42
Operator : SY/MD
Sample : PB134469TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB001

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.054	17.9	ug/L	166358	1	6.256	464947	50.0
Propanoic acid,...	8.742	21.5	ug/L	240828	2	9.426	560262	50.0
Butanoic acid, ...	9.224	13.2	ug/L	147877	2	9.426	560262	50.0