

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061219\
 Data File : VU032643.D
 Acq On : 12 Jun 2019 11:53
 Operator : JC/SP
 Sample : K3286-02
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JS4

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.180	24	28	38	rVB2	5521	5758	0.73%	0.077%
2	1.395	88	95	107	rBV	99920	102714	13.07%	1.382%
3	1.469	113	118	134	rVB	21201	23089	2.94%	0.311%
4	1.675	175	182	197	rVB	72406	87956	11.19%	1.183%
5	2.100	311	314	316	rBV	900	615	0.08%	0.008%
6	2.267	356	366	375	rBV	152699	230396	29.31%	3.100%
7	2.318	375	382	405	rVB	38391	62775	7.99%	0.845%
8	2.440	416	420	423	rBV3	730	677	0.09%	0.009%
9	2.627	468	478	481	rBV3	890	1391	0.18%	0.019%
10	2.698	491	500	511	rVB	6231	10325	1.31%	0.139%
11	2.836	539	543	547	rVB2	531	461	0.06%	0.006%
12	2.990	586	591	595	rVB4	308	367	0.05%	0.005%
13	3.186	641	652	665	rBV5	3942	8747	1.11%	0.118%
14	3.238	665	668	672	rVV2	316	290	0.04%	0.004%
15	3.421	715	725	741	rVV4	2182	5243	0.67%	0.071%
16	3.482	741	744	749	rVB2	280	267	0.03%	0.004%
17	3.530	756	759	764	rBV2	196	181	0.02%	0.002%
18	3.579	771	774	778	rVB	250	186	0.02%	0.003%
19	3.633	782	791	796	rBV4	771	1077	0.14%	0.014%
20	4.170	944	958	969	rBV	58818	146655	18.66%	1.973%
21	4.482	1050	1055	1058	rBV2	265	270	0.03%	0.004%
22	4.501	1058	1061	1068	rVB2	317	361	0.05%	0.005%
23	4.640	1087	1104	1129	rBV	107302	253296	32.22%	3.408%
24	4.771	1142	1145	1149	rVB3	362	241	0.03%	0.003%
25	4.820	1157	1160	1163	rVB2	268	179	0.02%	0.002%
26	4.839	1163	1166	1169	rVB	305	208	0.03%	0.003%
27	4.868	1169	1175	1176	rBV2	309	262	0.03%	0.004%
28	4.887	1176	1181	1189	rVB4	393	635	0.08%	0.009%
29	4.980	1208	1210	1213	rVV2	282	176	0.02%	0.002%
30	5.045	1226	1230	1234	rVB2	253	208	0.03%	0.003%
31	5.173	1267	1270	1276	rVB2	227	193	0.02%	0.003%
32	5.334	1298	1320	1350	rBV2	220219	641491	81.61%	8.631%
33	5.556	1379	1389	1407	rVB3	3181	7447	0.95%	0.100%
34	5.881	1452	1490	1510	rBV	213239	515612	65.59%	6.937%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\U061219\
 Data File : VU032643.D
 Acq On : 12 Jun 2019 11:53
 Operator : JC/SP
 Sample : K3286-02
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JS4

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
 Title : VOC Analysis

35	6.324	1615	1628	1645	rBV	145764	289442	36.82%	3.894%
36	6.421	1653	1658	1673	rVB2	4452	9001	1.15%	0.121%
37	6.578	1702	1707	1715	rBV2	2958	4038	0.51%	0.054%
38	6.697	1733	1744	1774	rBV	434997	786081	100.00%	10.576%
39	7.086	1862	1865	1869	rBV2	365	271	0.03%	0.004%
40	7.106	1869	1871	1875	rBV2	359	344	0.04%	0.005%
41	7.222	1895	1907	1924	rBV	84527	152881	19.45%	2.057%
42	7.373	1950	1954	1956	rBV2	249	199	0.03%	0.003%
43	7.414	1956	1967	1996	rBV	101073	177878	22.63%	2.393%
44	7.559	2000	2012	2031	rBV	300667	528539	67.24%	7.111%
45	7.771	2077	2078	2083	rBV3	350	264	0.03%	0.004%
46	7.845	2091	2101	2121	rBV	59643	105954	13.48%	1.426%
47	8.151	2182	2196	2213	rBV	57546	96444	12.27%	1.298%
48	8.257	2213	2229	2235	rVV2	20800	38037	4.84%	0.512%
49	8.305	2235	2244	2266	rVV	198054	356345	45.33%	4.794%
50	8.411	2267	2277	2304	rVV	320441	525692	66.88%	7.073%
51	8.524	2306	2312	2328	rVB2	10497	19688	2.50%	0.265%
52	8.810	2398	2401	2405	rVB3	249	208	0.03%	0.003%
53	8.900	2417	2429	2458	rBV	253768	406580	51.72%	5.470%
54	9.083	2470	2486	2510	rBV	293953	496114	63.11%	6.675%
55	9.430	2592	2594	2597	rBV	283	207	0.03%	0.003%
56	9.488	2608	2612	2618	rBV2	297	440	0.06%	0.006%
57	9.614	2643	2651	2659	rBV4	1849	3073	0.39%	0.041%
58	9.768	2691	2699	2712	rVV2	7972	13001	1.65%	0.175%
59	9.829	2716	2718	2722	rVV	478	237	0.03%	0.003%
60	9.942	2749	2753	2756	rBV2	184	191	0.02%	0.003%
61	10.019	2771	2777	2782	rBV2	218	277	0.04%	0.004%
62	10.128	2808	2811	2819	rBV2	295	281	0.04%	0.004%
63	10.212	2833	2837	2839	rBV	249	212	0.03%	0.003%
64	10.295	2859	2863	2867	rBV2	290	202	0.03%	0.003%
65	10.427	2891	2904	2926	rVV	205103	330483	42.04%	4.446%
66	10.607	2955	2960	2964	rVB4	732	831	0.11%	0.011%
67	10.678	2977	2982	2986	rBV2	319	249	0.03%	0.003%
68	10.710	2986	2992	2995	rVV2	219	211	0.03%	0.003%
69	10.771	3008	3011	3014	rBV2	314	220	0.03%	0.003%
70	10.839	3026	3032	3035	rBV2	181	220	0.03%	0.003%
71	10.935	3058	3062	3066	rBV3	231	185	0.02%	0.002%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061219\
 Data File : VU032643.D
 Acq On : 12 Jun 2019 11:53
 Operator : JC/SP
 Sample : K3286-02
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JS4

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
 Title : VOC Analysis

72	10.987	3075	3078	3082	rVB	311	180	0.02%	0.002%
73	11.006	3082	3084	3088	rVB2	292	196	0.02%	0.003%
74	11.032	3088	3092	3095	rBV2	251	189	0.02%	0.003%
75	11.057	3095	3100	3109	rVB3	332	493	0.06%	0.007%
76	11.180	3134	3138	3141	rBV	230	177	0.02%	0.002%
77	11.286	3167	3171	3174	rBV	200	209	0.03%	0.003%
78	11.479	3219	3231	3255	rBV	298355	484988	61.70%	6.525%
79	11.855	3331	3348	3373	rBV	290112	484617	61.65%	6.520%
80	12.205	3450	3457	3461	rVB3	447	431	0.05%	0.006%
81	12.479	3534	3542	3551	rBV4	917	1683	0.21%	0.023%
82	12.594	3574	3578	3583	rVB2	292	231	0.03%	0.003%
83	12.733	3615	3621	3622	rBV2	339	266	0.03%	0.004%
84	12.967	3690	3694	3695	rBV	268	191	0.02%	0.003%
85	13.035	3712	3715	3722	rVB2	225	269	0.03%	0.004%
86	13.077	3722	3728	3731	rBV2	374	443	0.06%	0.006%
87	13.147	3743	3750	3753	rBV2	338	393	0.05%	0.005%
88	13.286	3787	3793	3796	rBV2	274	243	0.03%	0.003%
89	13.379	3818	3822	3824	rBV	231	182	0.02%	0.002%
90	13.434	3834	3839	3841	rVB2	238	195	0.02%	0.003%
91	14.009	4014	4018	4023	rBV2	253	300	0.04%	0.004%
92	14.060	4031	4034	4037	rBV2	225	201	0.03%	0.003%
93	14.093	4040	4044	4048	rBV3	323	355	0.05%	0.005%
94	14.241	4086	4090	4092	rBV3	246	204	0.03%	0.003%
95	14.366	4126	4129	4131	rBV2	293	234	0.03%	0.003%
96	14.456	4152	4157	4160	rBV3	242	274	0.03%	0.004%
97	14.501	4168	4171	4175	rBV3	255	243	0.03%	0.003%
98	14.536	4180	4182	4190	rVB3	258	312	0.04%	0.004%
99	14.794	4260	4262	4265	rBV2	415	295	0.04%	0.004%
100	15.083	4347	4352	4354	rBV3	271	276	0.04%	0.004%

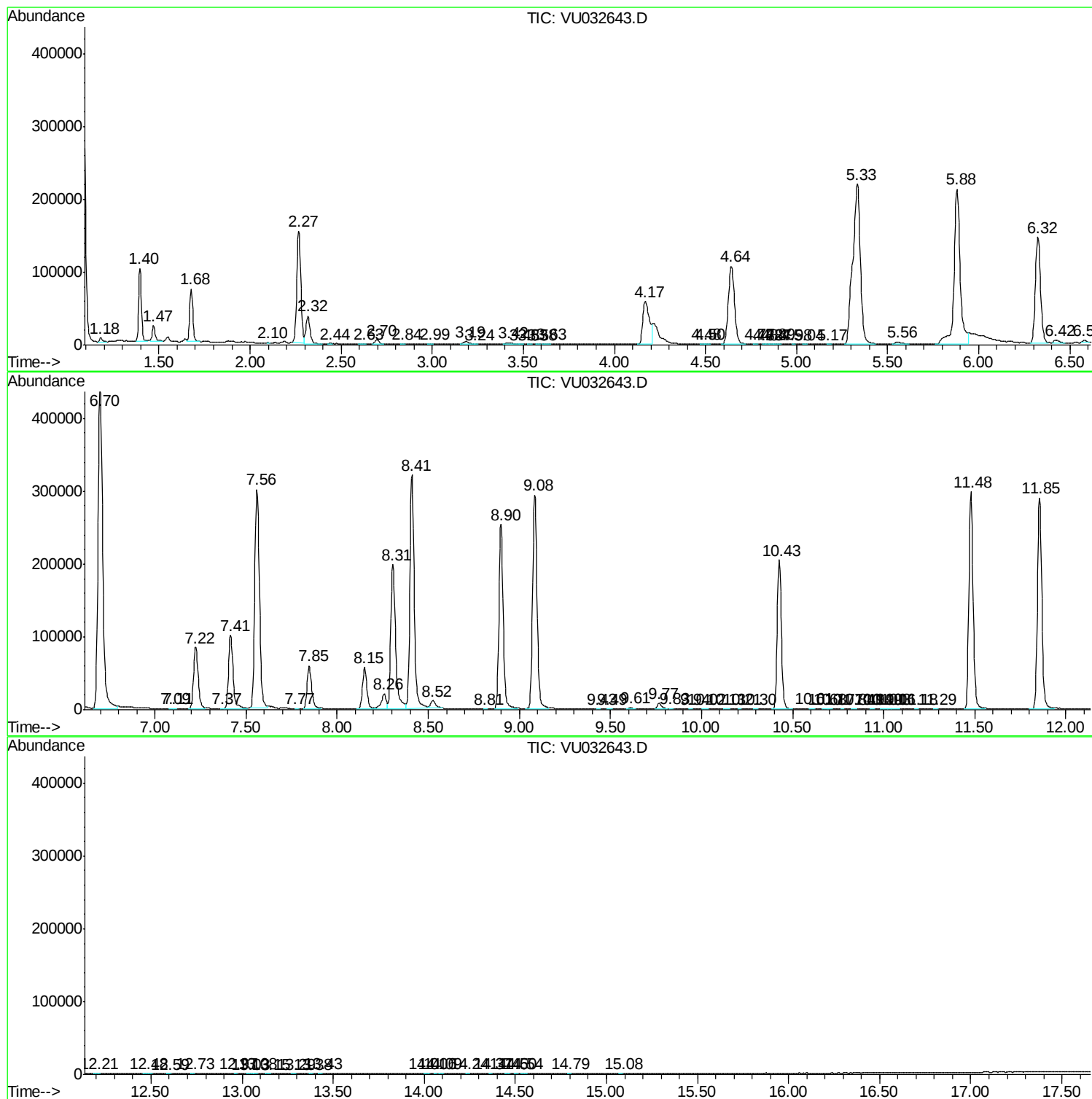
Sum of corrected areas: 7432539

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032643.D
Acq On : 12 Jun 2019 11:53
Operator : JC/SP
Sample : K3286-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JS4

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032643.D
Acq On : 12 Jun 2019 11:53
Operator : JC/SP
Sample : K3286-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JS4

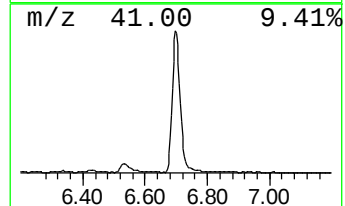
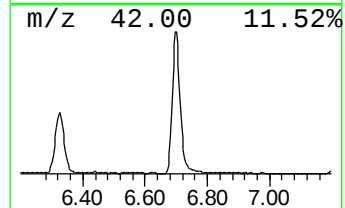
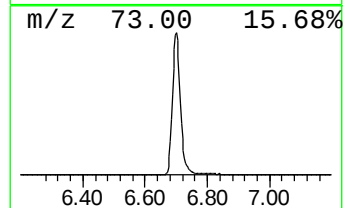
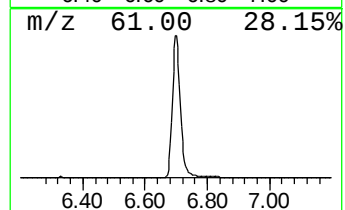
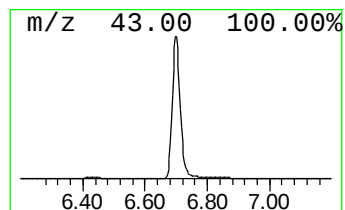
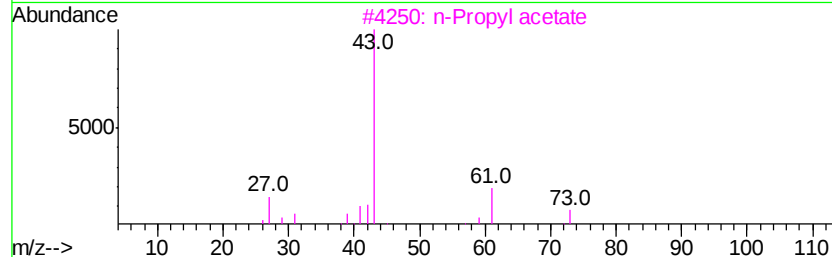
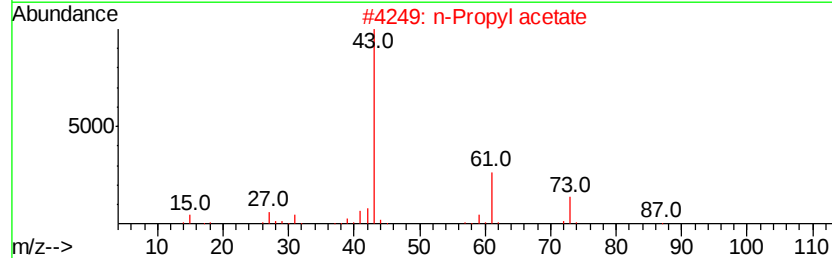
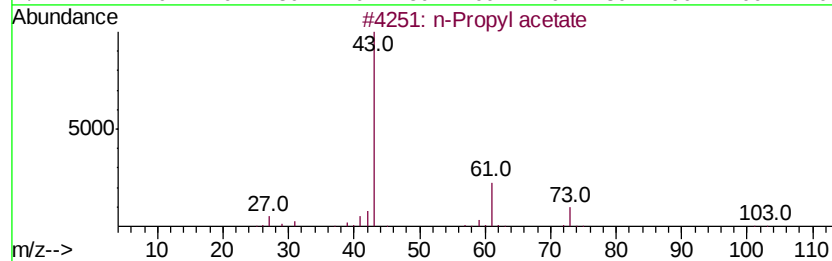
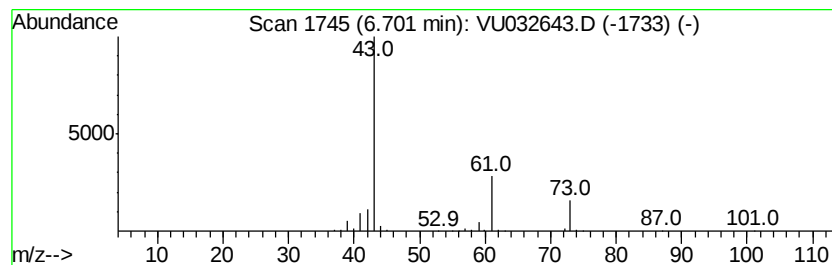
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	76.23 ug/L	786081	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	64
4		Isopropyl acetate	102	C5H10O2	000108-21-4	36
5		1-Butanamine	73	C4H11N	000109-73-9	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032643.D
Acq On : 12 Jun 2019 11:53
Operator : JC/SP
Sample : K3286-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JS4

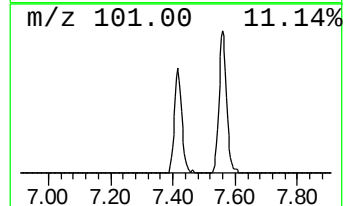
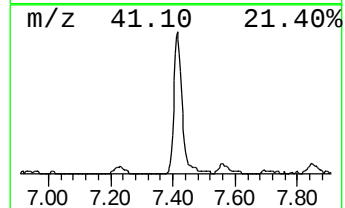
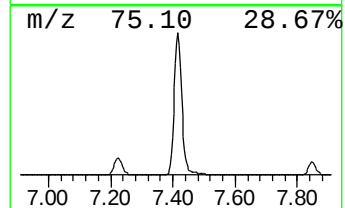
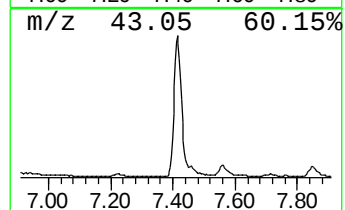
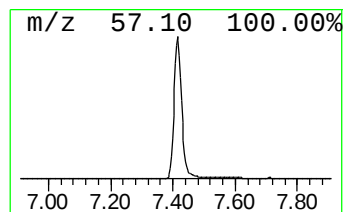
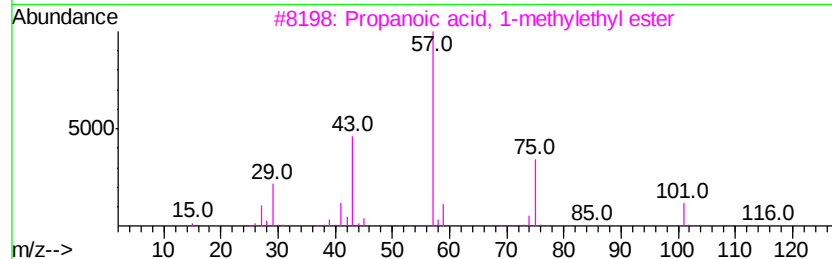
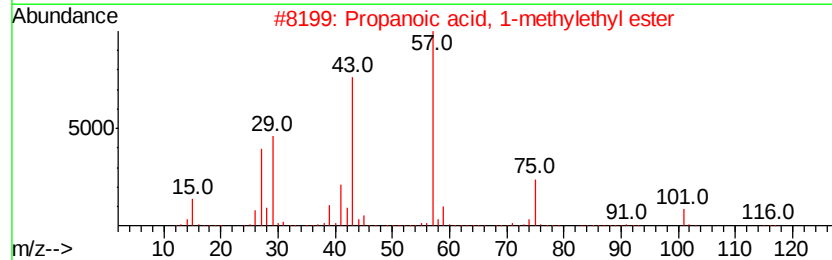
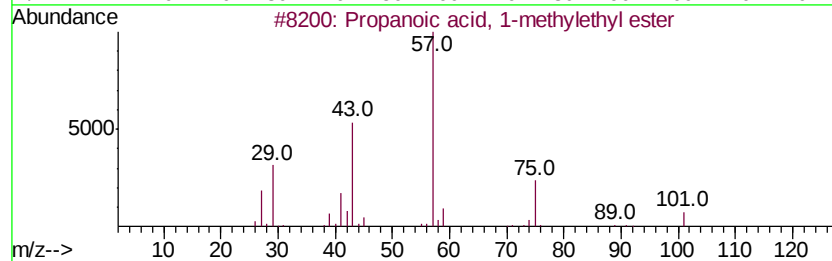
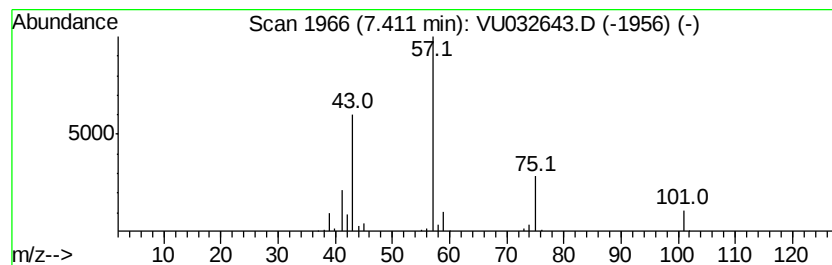
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	17.25 ug/L	177878	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
4		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032643.D
Acq On : 12 Jun 2019 11:53
Operator : JC/SP
Sample : K3286-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JS4

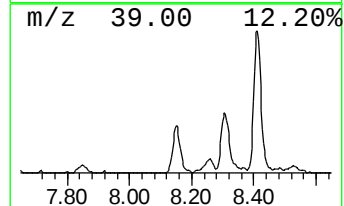
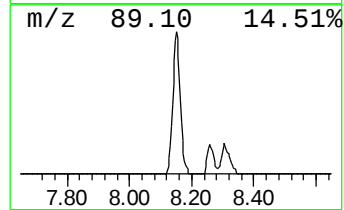
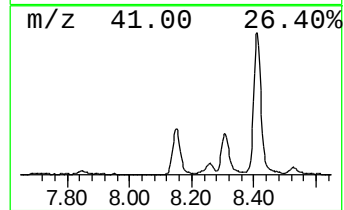
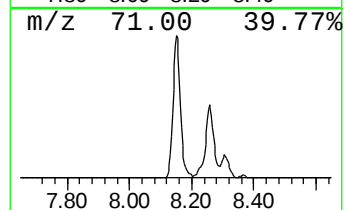
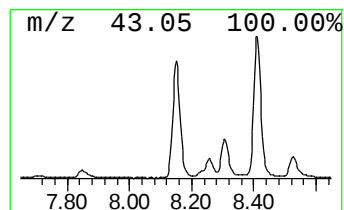
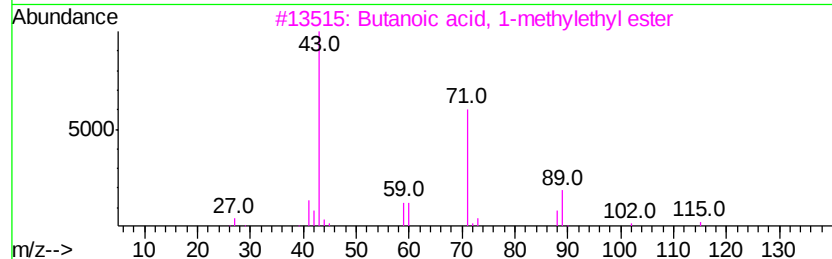
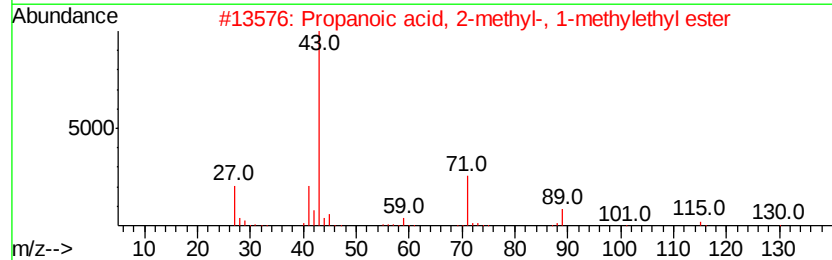
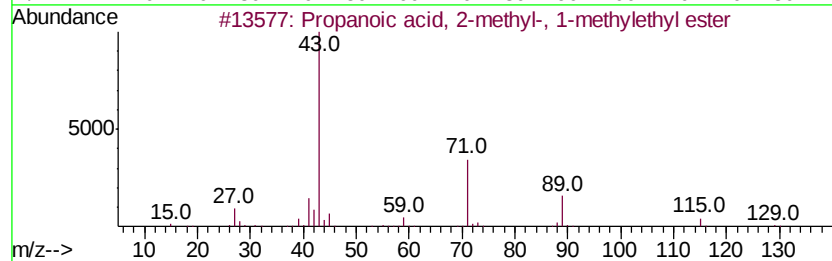
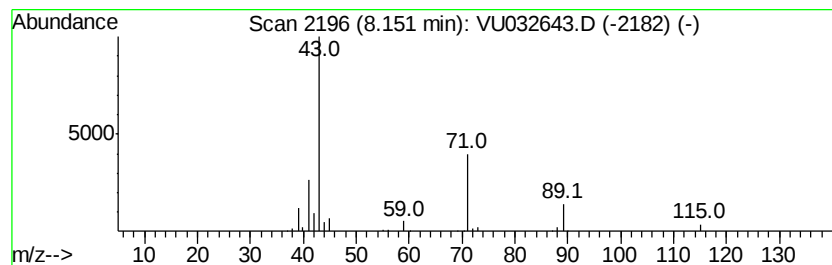
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	9.72 ug/L	96444	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
3		Butanoic acid, 1-methyl-ethyl ester	130	C7H14O2	000638-11-9	56
4		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	56
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032643.D
Acq On : 12 Jun 2019 11:53
Operator : JC/SP
Sample : K3286-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
C0JS4

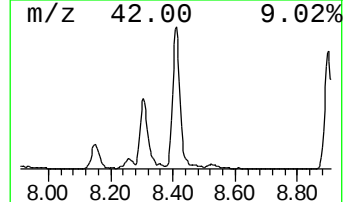
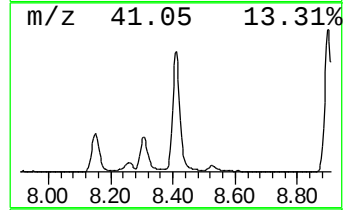
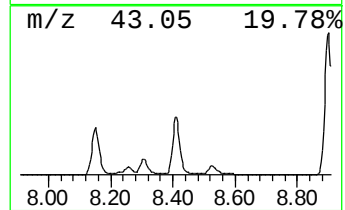
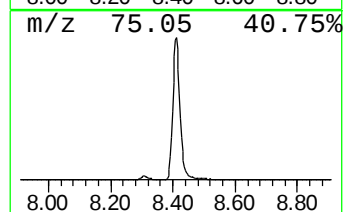
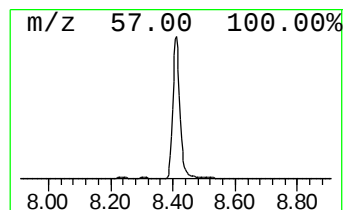
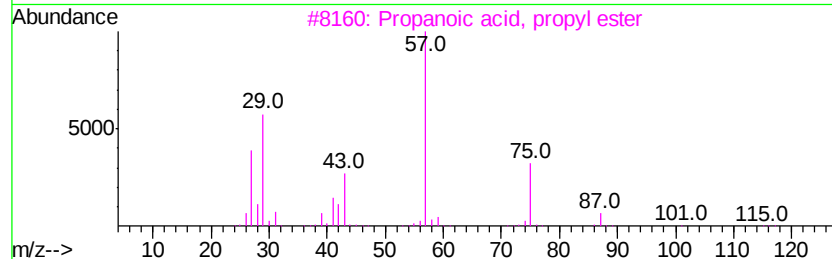
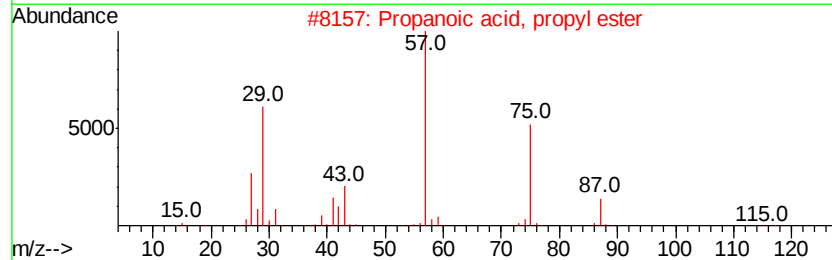
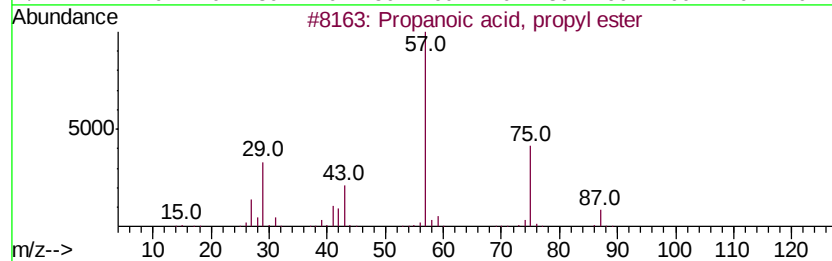
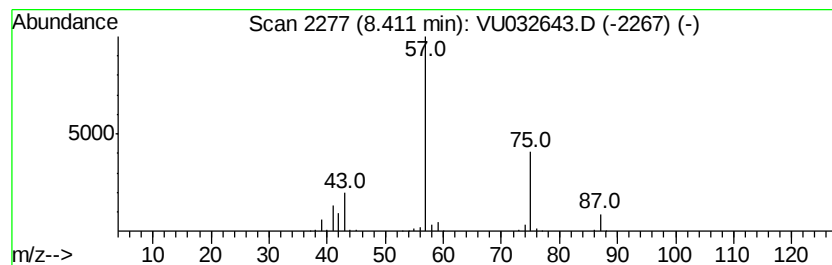
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	52.98 ug/L	525692	Chlorobenzene-d5	9.09

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	78	
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061219\
Data File : VU032643.D
Acq On : 12 Jun 2019 11:53
Operator : JC/SP
Sample : K3286-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 8 Sample Multiplier: 1

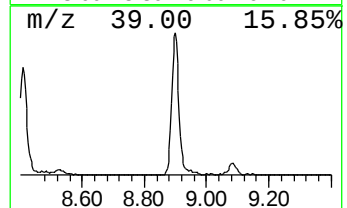
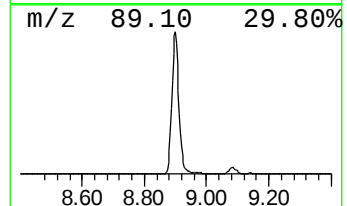
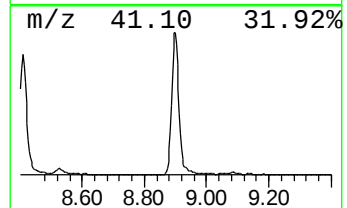
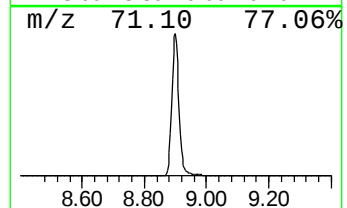
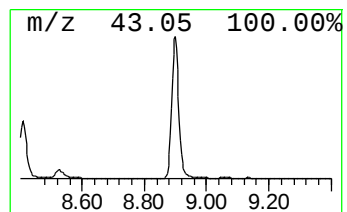
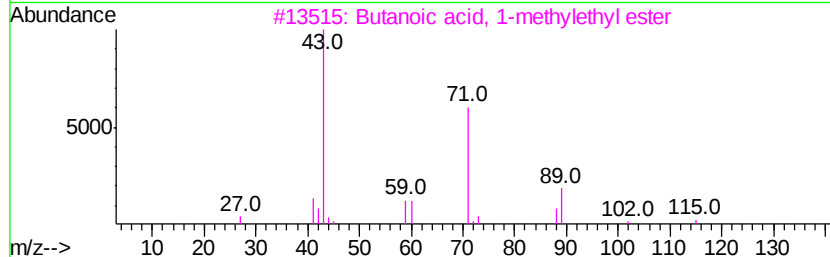
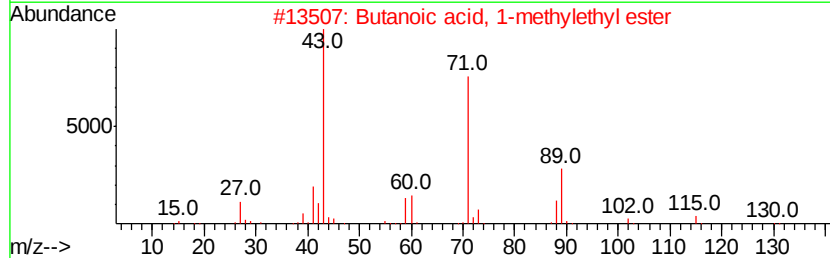
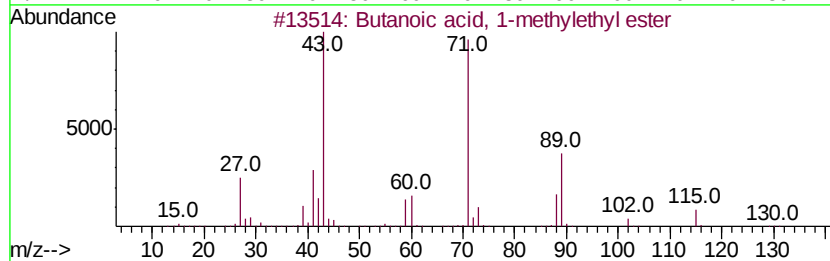
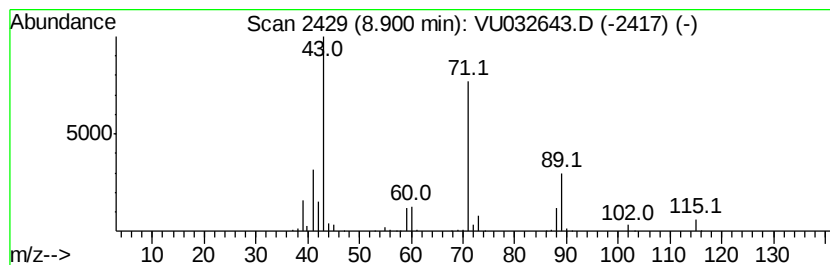
Instrument :
MSVOA_U
ClientSampleId :
C0JS4

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.90	40.98 ug/L	406580	Chlorobenzene-d5	9.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	83
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061219\
Data File : VU032643.D
Acq On : 12 Jun 2019 11:53
Operator : JC/SP
Sample : K3286-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JS4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.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	6.70	76.2	ug/L	786081	1	5.88	515612	50.0
Propanoic acid, 1...	7.41	17.3	ug/L	177878	1	5.88	515612	50.0
Propanoic acid, 2...	8.15	9.7	ug/L	96444	2	9.09	496114	50.0
Propanoic acid, p...	8.41	53.0	ug/L	525692	2	9.09	496114	50.0
Butanoic acid, 1-...	8.90	41.0	ug/L	406580	2	9.09	496114	50.0