

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
 Data File : VU025616.D
 Acq On : 23 Jul 2018 21:01
 Operator : MD/SY
 Sample : VLEB#03
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB#03

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\SOMULM072018WMA.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	0.825	67	73	75	rBV3	359	419	0.04%	0.004%
2	1.050	139	143	145	rBV	777	637	0.05%	0.006%
3	1.089	147	155	175	rBV	152468	174440	14.96%	1.541%
4	1.401	245	252	270	rVB	152069	158656	13.60%	1.402%
5	1.684	331	340	352	rBV	111880	138581	11.88%	1.224%
6	2.275	513	524	534	rBV	250618	378710	32.47%	3.346%
7	2.442	570	576	584	rBV3	3959	6277	0.54%	0.055%
8	2.619	619	631	642	rBV2	4428	7772	0.67%	0.069%
9	2.706	645	658	683	rVB	263456	470264	40.32%	4.155%
10	2.841	690	700	708	rVB7	1306	2918	0.25%	0.026%
11	2.876	708	711	716	rVB2	590	503	0.04%	0.004%
12	2.925	722	726	729	rBV4	480	472	0.04%	0.004%
13	3.175	801	804	808	rVB2	566	343	0.03%	0.003%
14	3.314	836	847	852	rBV7	1140	1933	0.17%	0.017%
15	3.442	884	887	894	rVB2	578	411	0.04%	0.004%
16	3.899	1025	1029	1037	rVB2	363	388	0.03%	0.003%
17	4.179	1099	1116	1141	rBV	109391	284340	24.38%	2.512%
18	4.381	1174	1179	1182	rBV5	703	750	0.06%	0.007%
19	4.487	1207	1212	1217	rVB3	568	601	0.05%	0.005%
20	4.655	1246	1264	1285	rBV	203153	478801	41.06%	4.230%
21	4.841	1318	1322	1331	rVB2	432	595	0.05%	0.005%
22	4.892	1331	1338	1347	rVB3	1040	1611	0.14%	0.014%
23	4.992	1363	1369	1372	rBV3	538	545	0.05%	0.005%
24	5.346	1454	1479	1507	rBV2	391009	1166207	100.00%	10.304%
25	5.552	1528	1543	1565	rVV2	96512	199562	17.11%	1.763%
26	5.892	1625	1649	1664	rBV	388284	820124	70.32%	7.246%
27	6.336	1773	1787	1805	rVB	265377	523655	44.90%	4.627%
28	6.709	1891	1903	1937	rVB	144888	262826	22.54%	2.322%
29	7.230	2053	2065	2087	rBV	159001	281333	24.12%	2.486%
30	7.314	2088	2091	2096	rVB3	974	724	0.06%	0.006%
31	7.423	2117	2125	2135	rBV4	5895	9848	0.84%	0.087%
32	7.568	2156	2170	2198	rBV	555873	971353	83.29%	8.582%
33	7.854	2247	2259	2276	rBV	114604	196483	16.85%	1.736%
34	8.005	2304	2306	2311	rBV2	469	408	0.03%	0.004%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
 Data File : VU025616.D
 Acq On : 23 Jul 2018 21:01
 Operator : MD/SY
 Sample : VLEB#03
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB#03

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\SOMULM072018WMA.M
 Title : VOC Analysis

35	8.043	2316	2318	2321	rVB2	726	391	0.03%	0.003%
36	8.188	2344	2363	2371	rBV4	11082	29537	2.53%	0.261%
37	8.314	2392	2402	2420	rVB	371937	618420	53.03%	5.464%
38	8.420	2425	2435	2450	rVB	72335	114210	9.79%	1.009%
39	8.526	2460	2468	2484	rVB2	20425	33884	2.91%	0.299%
40	8.838	2563	2565	2570	rVB3	685	458	0.04%	0.004%
41	8.905	2576	2586	2603	rBV	79481	124801	10.70%	1.103%
42	8.976	2603	2608	2613	rBV3	521	502	0.04%	0.004%
43	9.092	2628	2644	2669	rVV	531154	884657	75.86%	7.816%
44	9.256	2688	2695	2703	rVB4	3032	4308	0.37%	0.038%
45	9.378	2729	2733	2742	rVB5	1880	2691	0.23%	0.024%
46	9.564	2788	2791	2797	rBV3	456	511	0.04%	0.005%
47	9.728	2836	2842	2845	rBV5	474	608	0.05%	0.005%
48	9.773	2848	2856	2859	rBV4	2669	3778	0.32%	0.033%
49	9.886	2887	2891	2893	rBV2	410	379	0.03%	0.003%
50	10.085	2949	2953	2958	rBV5	449	558	0.05%	0.005%
51	10.172	2977	2980	2983	rVV2	829	503	0.04%	0.004%
52	10.230	2993	2998	3002	rBV3	713	924	0.08%	0.008%
53	10.436	3049	3062	3087	rBV	381880	607556	52.10%	5.368%
54	10.690	3135	3141	3144	rBV3	934	1006	0.09%	0.009%
55	10.776	3161	3168	3174	rVB3	1928	2615	0.22%	0.023%
56	10.982	3227	3232	3238	rVV2	835	1126	0.10%	0.010%
57	11.082	3261	3263	3268	rVB2	578	361	0.03%	0.003%
58	11.153	3276	3285	3295	rBV3	3650	5454	0.47%	0.048%
59	11.420	3366	3368	3374	rBV3	569	468	0.04%	0.004%
60	11.487	3376	3389	3408	rBV	589898	920711	78.95%	8.135%
61	11.574	3413	3416	3426	rVB3	2293	2382	0.20%	0.021%
62	11.699	3451	3455	3456	rBV	469	374	0.03%	0.003%
63	11.770	3468	3477	3487	rBV2	10302	15951	1.37%	0.141%
64	11.863	3493	3506	3525	rBV	599396	947932	81.28%	8.375%
65	11.985	3535	3544	3554	rVB6	2078	3840	0.33%	0.034%
66	12.030	3554	3558	3562	rBV3	567	565	0.05%	0.005%
67	12.117	3583	3585	3590	rBV3	480	415	0.04%	0.004%
68	12.217	3612	3616	3617	rBV2	410	331	0.03%	0.003%
69	12.256	3621	3628	3635	rVV3	3750	5121	0.44%	0.045%
70	12.326	3647	3650	3653	rBV2	488	363	0.03%	0.003%
71	12.362	3653	3661	3667	rVV4	2179	3300	0.28%	0.029%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072318\
 Data File : VU025616.D
 Acq On : 23 Jul 2018 21:01
 Operator : MD/SY
 Sample : VLEB#03
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB#03

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\SOMULM072018WMA.M
 Title : VOC Analysis

72	12.481	3693	3698	3702	rBV4	1349	1401	0.12%	0.012%
73	12.542	3712	3717	3718	rBV2	576	528	0.05%	0.005%
74	12.651	3745	3751	3759	rVB5	2966	4698	0.40%	0.042%
75	12.706	3764	3768	3772	rVB4	1061	1043	0.09%	0.009%
76	12.764	3783	3786	3788	rBV	758	400	0.03%	0.004%
77	12.870	3815	3819	3821	rBV3	496	387	0.03%	0.003%
78	12.966	3844	3849	3858	rVB4	2745	4332	0.37%	0.038%
79	13.124	3890	3898	3908	rVB4	10843	16325	1.40%	0.144%
80	13.169	3909	3912	3914	rVV3	823	610	0.05%	0.005%
81	13.191	3915	3919	3927	rVB4	2598	2917	0.25%	0.026%
82	13.297	3943	3952	3959	rVB6	6053	8993	0.77%	0.079%
83	13.461	3996	4003	4010	rVB7	2370	3385	0.29%	0.030%
84	13.509	4012	4018	4027	rBV9	3541	5401	0.46%	0.048%
85	13.609	4046	4049	4051	rBV2	1142	715	0.06%	0.006%
86	13.638	4056	4058	4065	rVB5	1654	1533	0.13%	0.014%
87	13.747	4081	4092	4110	rBV	108605	179009	15.35%	1.582%
88	13.866	4119	4129	4138	rVB10	3514	6095	0.52%	0.054%
89	13.953	4153	4156	4165	rVB7	2173	2680	0.23%	0.024%
90	14.156	4214	4219	4228	rVB7	2351	3727	0.32%	0.033%
91	14.220	4237	4239	4244	rBV2	593	479	0.04%	0.004%
92	14.278	4254	4257	4259	rBV3	772	474	0.04%	0.004%
93	14.355	4269	4281	4288	rBV6	6489	13510	1.16%	0.119%
94	14.551	4333	4342	4348	rBV6	1957	3565	0.31%	0.031%
95	14.680	4377	4382	4389	rVB6	3433	4069	0.35%	0.036%
96	14.728	4395	4397	4399	rBV2	579	325	0.03%	0.003%
97	14.882	4435	4445	4457	rBV	29993	51556	4.42%	0.456%
98	15.066	4491	4502	4517	rBV	31616	55779	4.78%	0.493%
99	16.066	4806	4813	4820	rBV6	12912	20103	1.72%	0.178%
100	16.744	5017	5024	5036	rVB	24744	41031	3.52%	0.363%

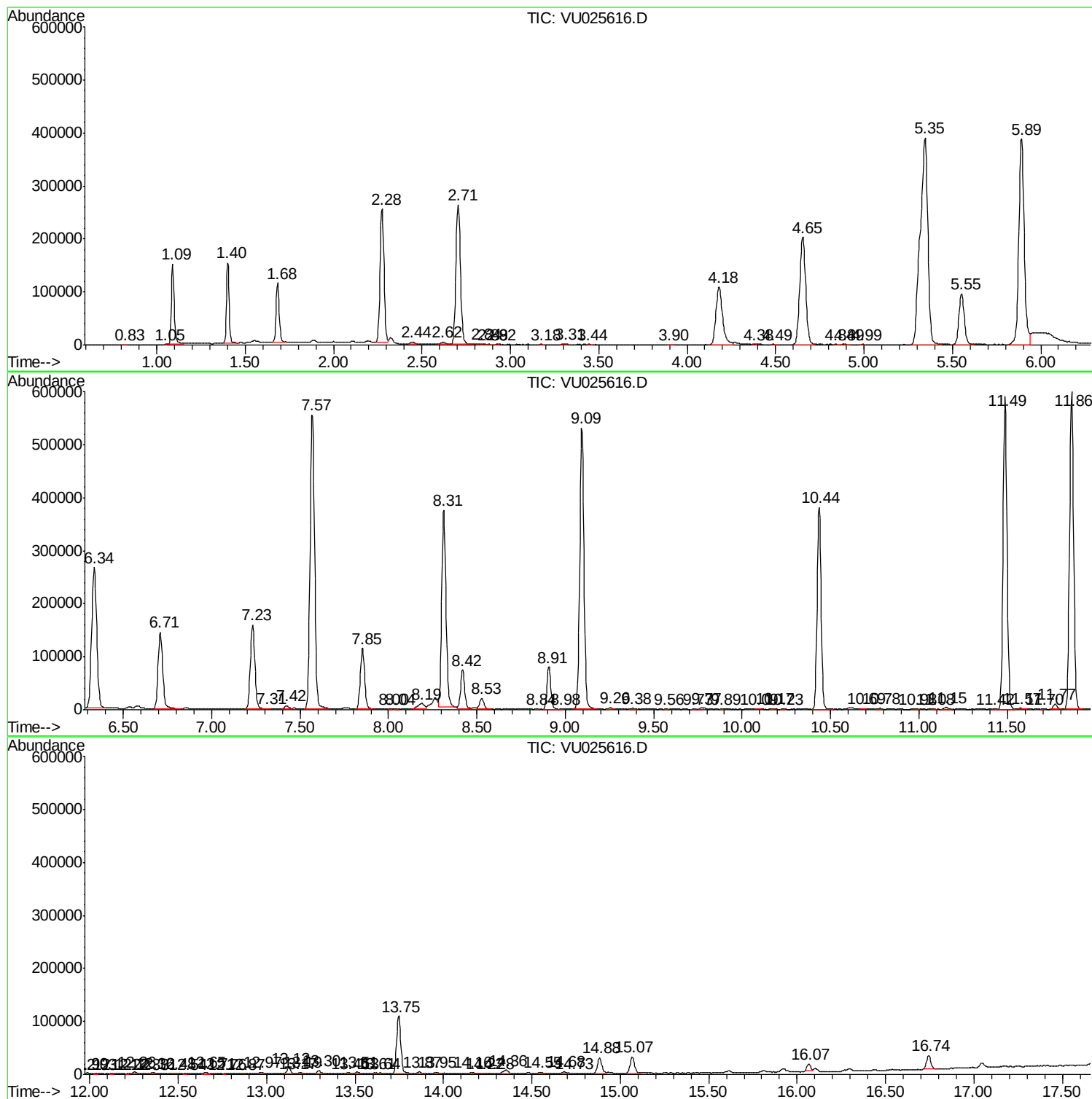
Sum of corrected areas: 11318551

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025616.D
Acq On : 23 Jul 2018 21:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB#03

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025616.D
Acq On : 23 Jul 2018 21:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB#03

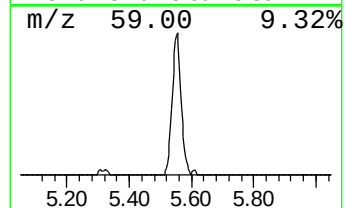
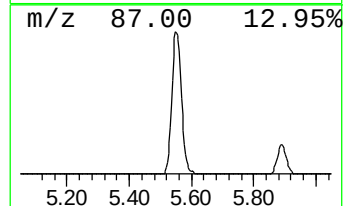
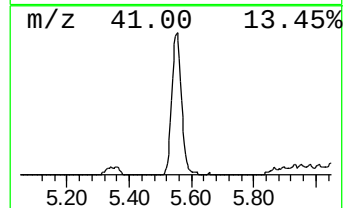
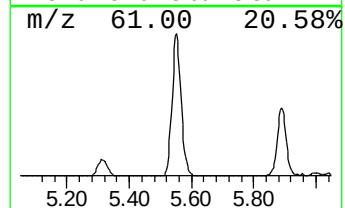
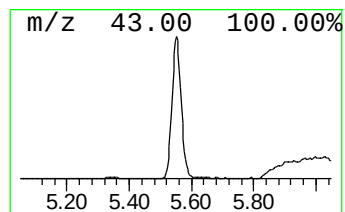
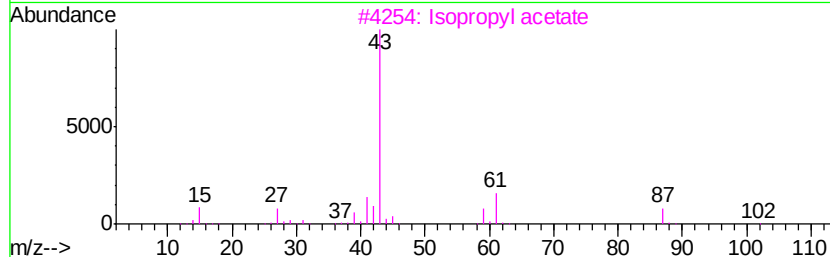
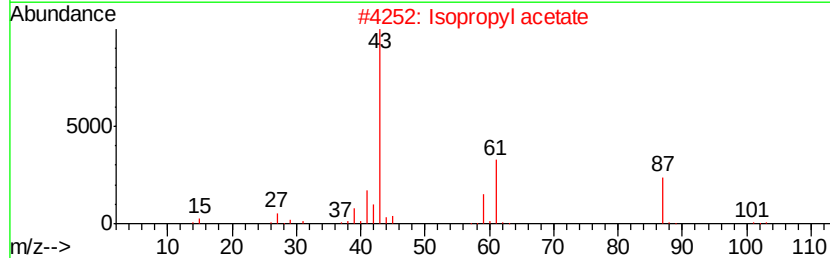
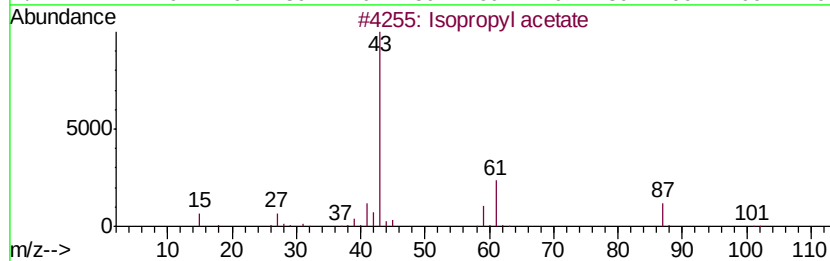
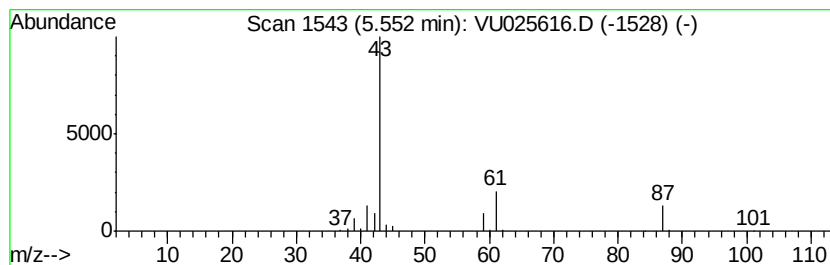
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.55	12.17 ug/L	199562	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl acetate	102	C5H10O2	000108-21-4	83
2		Isopropyl acetate	102	C5H10O2	000108-21-4	64
3		Isopropyl acetate	102	C5H10O2	000108-21-4	64
4		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	28
5		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	28



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025616.D
Acq On : 23 Jul 2018 21:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB#03

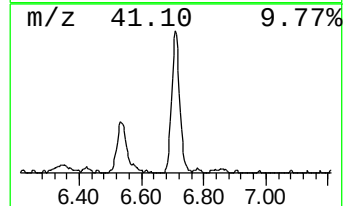
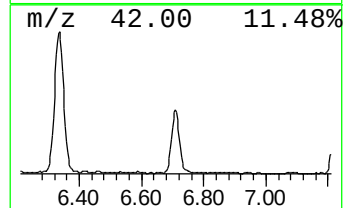
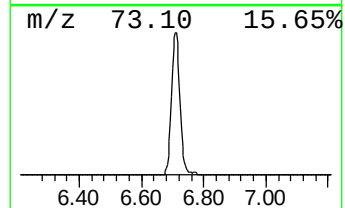
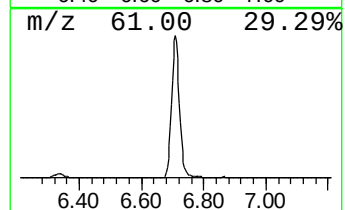
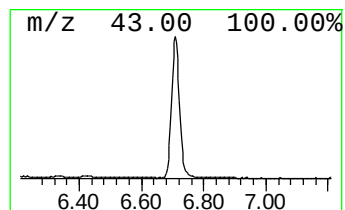
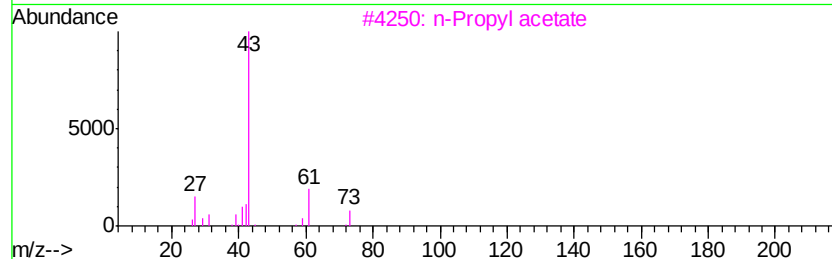
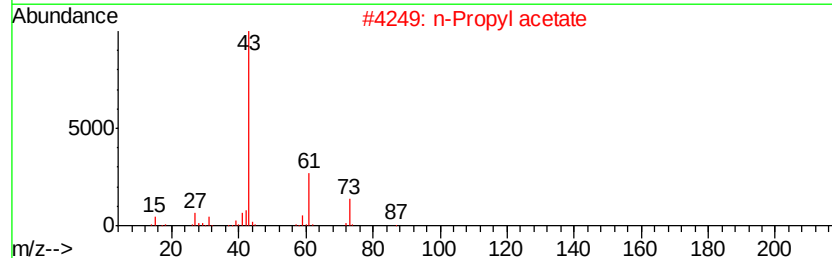
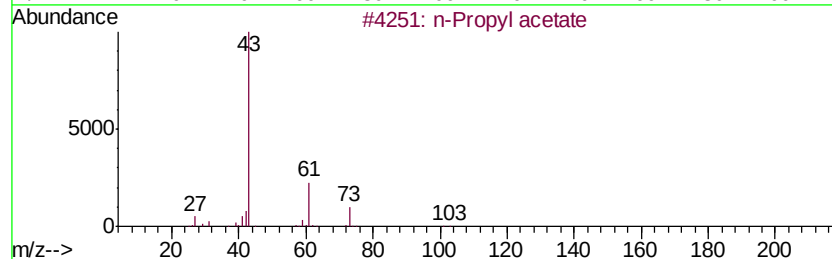
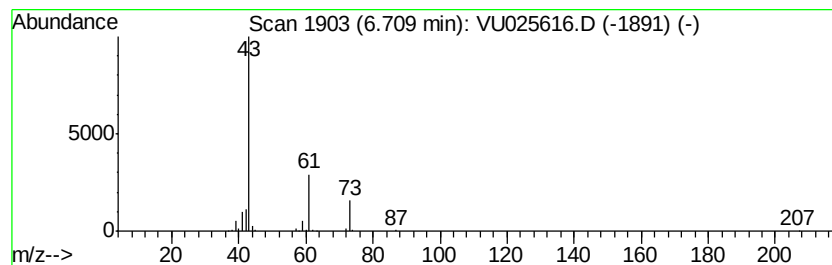
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	16.02 ug/L	262826	1,4-Difluorobenzene	5.89

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	45
4		Isopropyl acetate	102	C5H10O2	000108-21-4	9
5		Isopropyl acetate	102	C5H10O2	000108-21-4	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025616.D
Acq On : 23 Jul 2018 21:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB#03

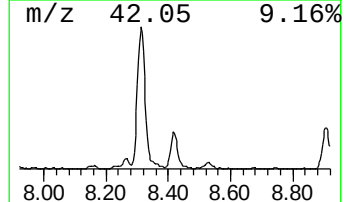
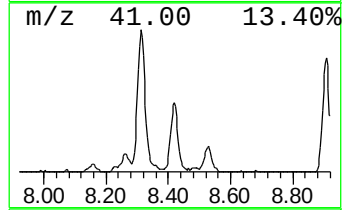
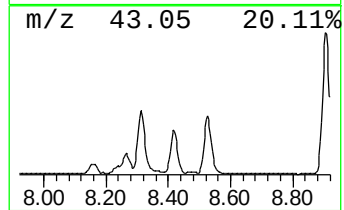
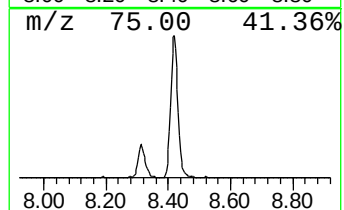
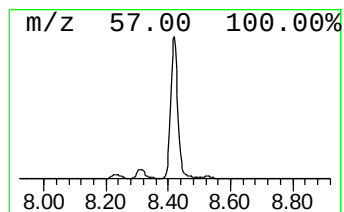
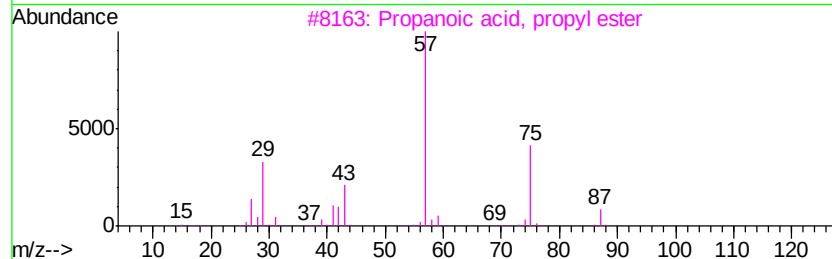
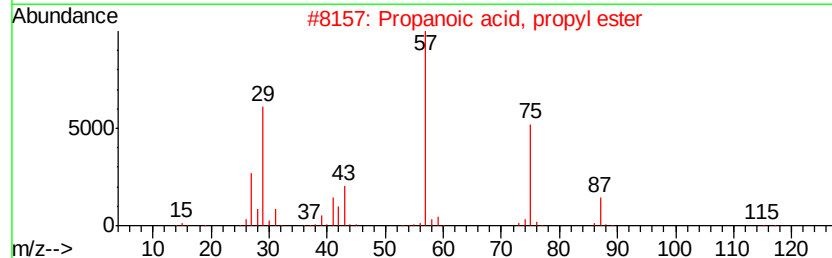
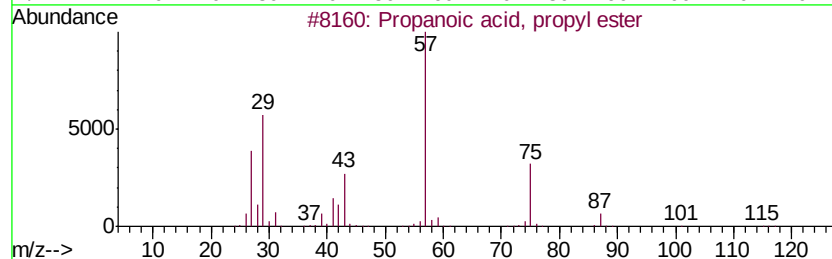
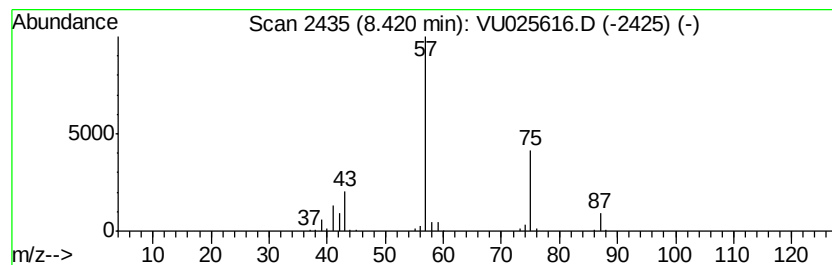
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	6.46 ug/L	114210	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	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025616.D
Acq On : 23 Jul 2018 21:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB#03

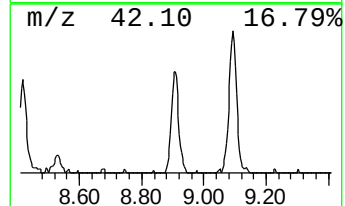
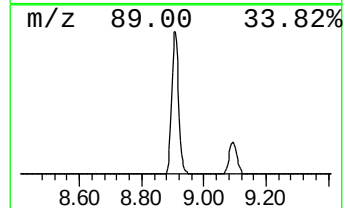
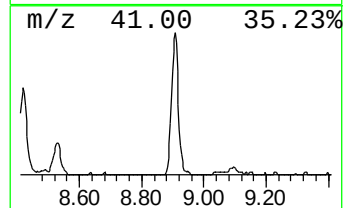
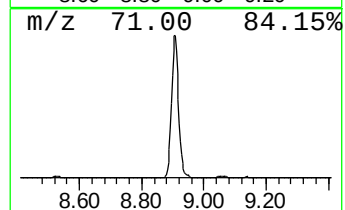
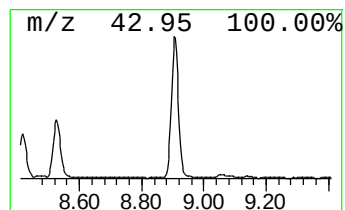
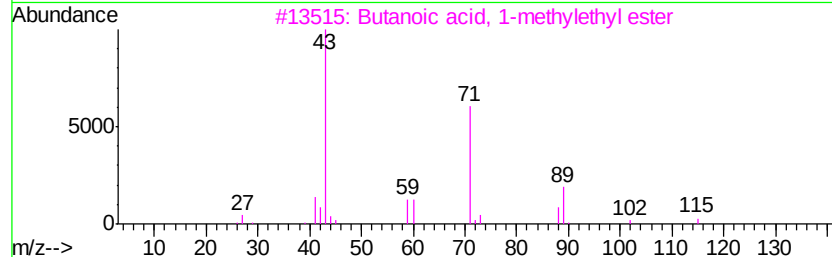
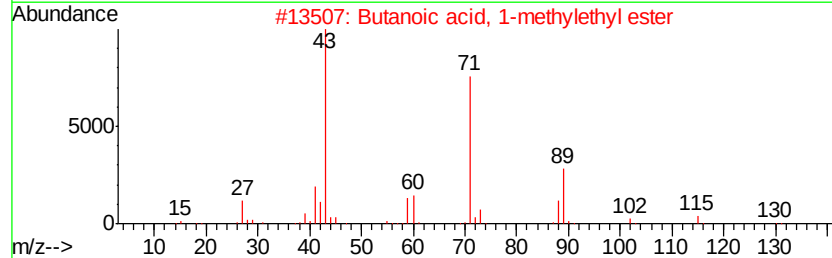
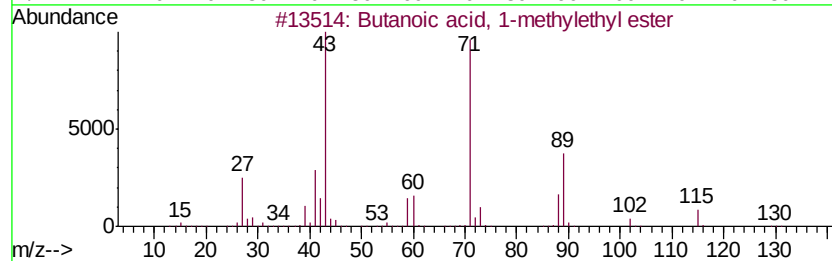
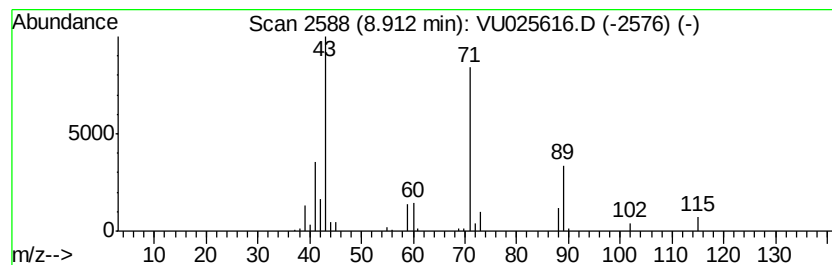
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.91	7.05 ug/L	124801	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	78
4		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	72
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU072318\
Data File : VU025616.D
Acq On : 23 Jul 2018 21:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB#03

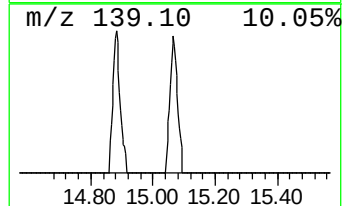
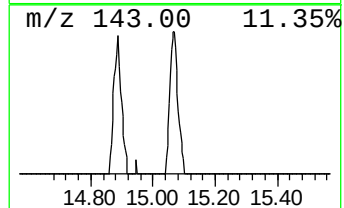
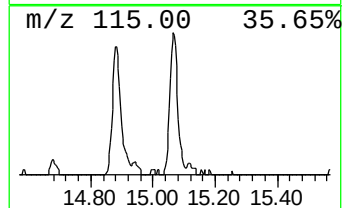
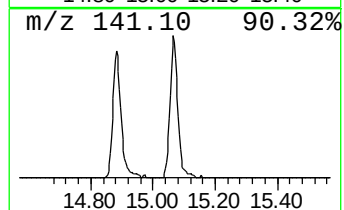
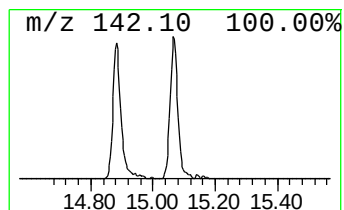
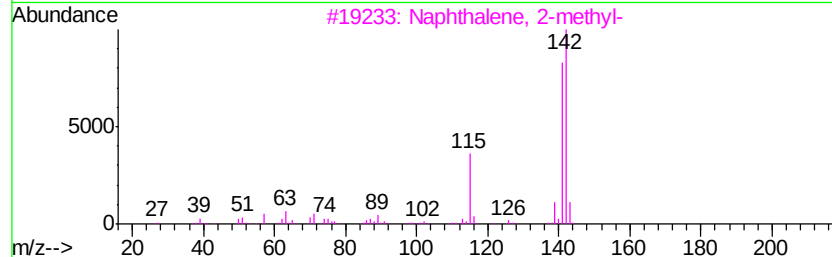
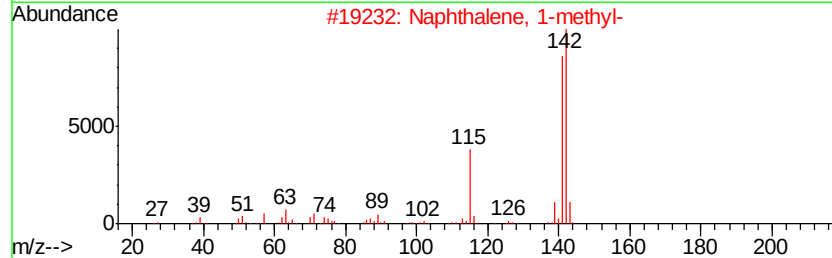
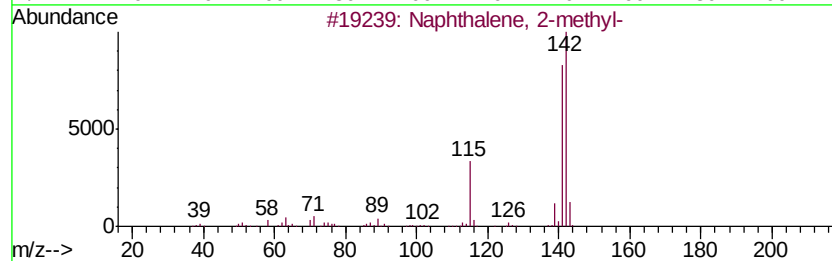
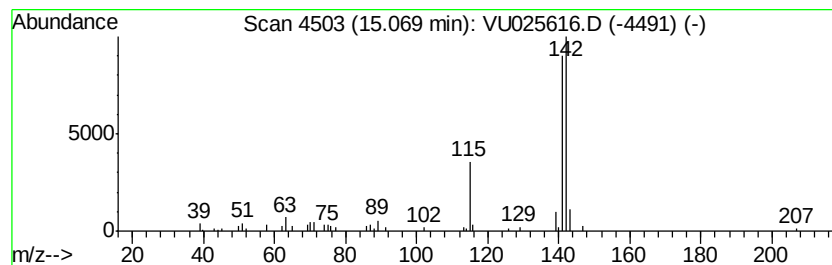
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	3.03 ug/L	55779	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5		Benzocycloheptatriene	142	C11H10	000264-09-5	91



Data Path : Z:\V0ASRV\HPCHEM1\MSV0A_U\DATA\VU072318\
Data File : VU025616.D
Acq On : 23 Jul 2018 21:01
Operator : MD/SY
Sample : VLEB#03
Misc : 5.0mL/MSV0A_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSV0A_U
ClientSampleId :
VLEB#03

Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_U\METHOD\SOMULM072018WMA.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
Isopropyl acetate	5.55	12.2	ug/L	199562	1	5.89	820124	50.0
n-Propyl acetate	6.71	16.0	ug/L	262826	1	5.89	820124	50.0
Propanoic acid, p...	8.42	6.5	ug/L	114210	2	9.09	884657	50.0
Butanoic acid, 1-...	8.91	7.0	ug/L	124801	2	9.09	884657	50.0
Naphthalene, 1-me...	15.07	3.0	ug/L	55779	3	11.49	920711	50.0