

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072318\
 Data File : VU025615.D
 Acq On : 23 Jul 2018 20:38
 Operator : MD/SY
 Sample : VLEB02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB02

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	0.619	6	9	11	rBV2	168	107	0.01%	0.001%
2	0.632	11	13	15	rBV2	238	156	0.01%	0.001%
3	0.725	38	42	45	rBV	282	239	0.02%	0.002%
4	0.757	50	52	58	rBV2	184	213	0.02%	0.002%
5	0.812	63	69	71	rBV3	321	242	0.02%	0.002%
6	0.828	71	74	78	rBV	280	269	0.02%	0.002%
7	0.934	103	107	108	rBV2	214	166	0.01%	0.001%
8	0.989	122	124	127	rVB	218	120	0.01%	0.001%
9	1.005	127	129	132	rBV2	241	161	0.01%	0.001%
10	1.089	148	155	171	rBV	153188	173033	14.33%	1.513%
11	1.400	245	252	265	rBV	158088	165154	13.68%	1.444%
12	1.683	333	340	354	rVB	117344	147475	12.22%	1.290%
13	2.275	514	524	534	rBV	268402	398261	32.99%	3.483%
14	2.706	645	658	678	rBV	271573	481672	39.90%	4.212%
15	3.130	786	790	796	rVB3	429	405	0.03%	0.004%
16	3.159	796	799	803	rVB2	302	213	0.02%	0.002%
17	3.191	805	809	812	rBV2	412	323	0.03%	0.003%
18	3.230	819	821	822	rBV	144	49	0.00%	0.000%
19	3.243	822	825	827	rVV2	253	179	0.01%	0.002%
20	3.275	831	835	837	rBV	245	176	0.01%	0.002%
21	3.310	838	846	850	rVV4	1181	1756	0.15%	0.015%
22	3.346	854	857	859	rBV2	334	239	0.02%	0.002%
23	3.391	866	871	873	rBV	457	435	0.04%	0.004%
24	3.436	883	885	886	rBV	484	197	0.02%	0.002%
25	3.471	894	896	897	rVB	101	21	0.00%	0.000%
26	3.481	897	899	900	rBV	230	110	0.01%	0.001%
27	3.568	923	926	931	rBV3	331	312	0.03%	0.003%
28	3.616	938	941	944	rBV2	409	249	0.02%	0.002%
29	3.638	944	948	950	rBV2	356	278	0.02%	0.002%
30	3.757	981	985	987	rBV	348	213	0.02%	0.002%
31	3.809	996	1001	1007	rBV3	415	473	0.04%	0.004%
32	3.924	1035	1037	1041	rBV2	245	186	0.02%	0.002%
33	3.944	1041	1043	1046	rBV2	130	85	0.01%	0.001%
34	4.098	1089	1091	1092	rBV	285	138	0.01%	0.001%

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 ClientSampleId :
 VLEB02

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
 Title : VOC Analysis

35	4.178	1102	1116	1138	rBV2	110029	282615	23.41%	2.472%
36	4.494	1212	1214	1216	rBV	72	40	0.00%	0.000%
37	4.506	1216	1218	1220	rBV	320	155	0.01%	0.001%
38	4.555	1228	1233	1235	rBV2	283	250	0.02%	0.002%
39	4.580	1239	1241	1242	rBV	128	31	0.00%	0.000%
40	4.590	1242	1244	1245	rBV	283	96	0.01%	0.001%
41	4.654	1245	1264	1289	rBV	209670	492105	40.76%	4.304%
42	4.860	1324	1328	1330	rBV2	316	235	0.02%	0.002%
43	4.883	1330	1335	1336	rBV2	701	613	0.05%	0.005%
44	4.982	1363	1366	1368	rBV2	320	222	0.02%	0.002%
45	5.079	1394	1396	1400	rBV2	217	124	0.01%	0.001%
46	5.162	1418	1422	1424	rBV	251	160	0.01%	0.001%
47	5.201	1432	1434	1436	rVB3	314	143	0.01%	0.001%
48	5.217	1436	1439	1440	rBV2	126	66	0.01%	0.001%
49	5.346	1454	1479	1508	rBV2	408562	1207322	100.00%	10.559%
50	5.551	1529	1543	1563	rBV	98822	201391	16.68%	1.761%
51	5.748	1601	1604	1606	rVB3	503	280	0.02%	0.002%
52	5.812	1621	1624	1630	rBV4	392	363	0.03%	0.003%
53	5.892	1630	1649	1666	rBV	399583	826934	68.49%	7.232%
54	6.336	1774	1787	1805	rVB	269280	534810	44.30%	4.677%
55	6.709	1892	1903	1930	rVB	145224	260397	21.57%	2.277%
56	7.230	2053	2065	2082	rBV	162689	287697	23.83%	2.516%
57	7.423	2118	2125	2133	rBV3	6052	9592	0.79%	0.084%
58	7.571	2156	2171	2188	rBV	572548	1000408	82.86%	8.749%
59	7.854	2247	2259	2282	rBV	121326	205552	17.03%	1.798%
60	8.027	2304	2313	2316	rBV5	709	1156	0.10%	0.010%
61	8.108	2335	2338	2342	rBV2	603	559	0.05%	0.005%
62	8.313	2393	2402	2424	rVB	372023	624785	51.75%	5.464%
63	8.419	2427	2435	2447	rVB	72253	113127	9.37%	0.989%
64	8.908	2576	2587	2603	rBV	82719	126333	10.46%	1.105%
65	9.091	2632	2644	2672	rVB	549997	910051	75.38%	7.959%
66	9.255	2689	2695	2703	rVB4	2738	3648	0.30%	0.032%
67	9.503	2768	2772	2777	rBV	718	545	0.05%	0.005%
68	9.554	2786	2788	2790	rBV	529	315	0.03%	0.003%
69	9.596	2798	2801	2806	rBV3	543	604	0.05%	0.005%
70	9.776	2848	2857	2867	rBV8	3460	6667	0.55%	0.058%
71	9.956	2911	2913	2914	rBV	460	234	0.02%	0.002%

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Integration Parameters: LSCINT.P

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 Title : VOC Analysis

72	10.281	3009	3014	3016	rBV	300	333	0.03%	0.003%
73	10.304	3019	3021	3022	rBV	294	123	0.01%	0.001%
74	10.435	3050	3062	3080	rBV	382436	605540	50.16%	5.296%
75	10.860	3193	3194	3195	rBV	252	63	0.01%	0.001%
76	11.114	3269	3273	3277	rBV4	686	631	0.05%	0.006%
77	11.152	3279	3285	3294	rVB3	4519	5969	0.49%	0.052%
78	11.210	3299	3303	3305	rBV2	498	387	0.03%	0.003%
79	11.423	3365	3369	3371	rBV2	1012	671	0.06%	0.006%
80	11.487	3377	3389	3409	rBV	620125	955474	79.14%	8.356%
81	11.770	3469	3477	3489	rVB3	10391	16569	1.37%	0.145%
82	11.863	3494	3506	3524	rVV	614523	976225	80.86%	8.538%
83	12.252	3622	3627	3634	rBV4	4070	5055	0.42%	0.044%
84	12.361	3652	3661	3664	rBV6	3167	4284	0.35%	0.037%
85	12.487	3693	3700	3705	rBV5	1829	2486	0.21%	0.022%
86	13.075	3879	3883	3885	rBV2	955	715	0.06%	0.006%
87	13.123	3892	3898	3910	rVB4	12604	17361	1.44%	0.152%
88	13.294	3946	3951	3965	rVB6	5711	9178	0.76%	0.080%
89	13.509	4013	4018	4025	rVB8	3508	4783	0.40%	0.042%
90	13.744	4081	4091	4113	rBV	139913	232970	19.30%	2.037%
91	14.882	4437	4445	4457	rBV2	29325	48709	4.03%	0.426%
92	15.065	4493	4502	4517	rVB	43819	73901	6.12%	0.646%

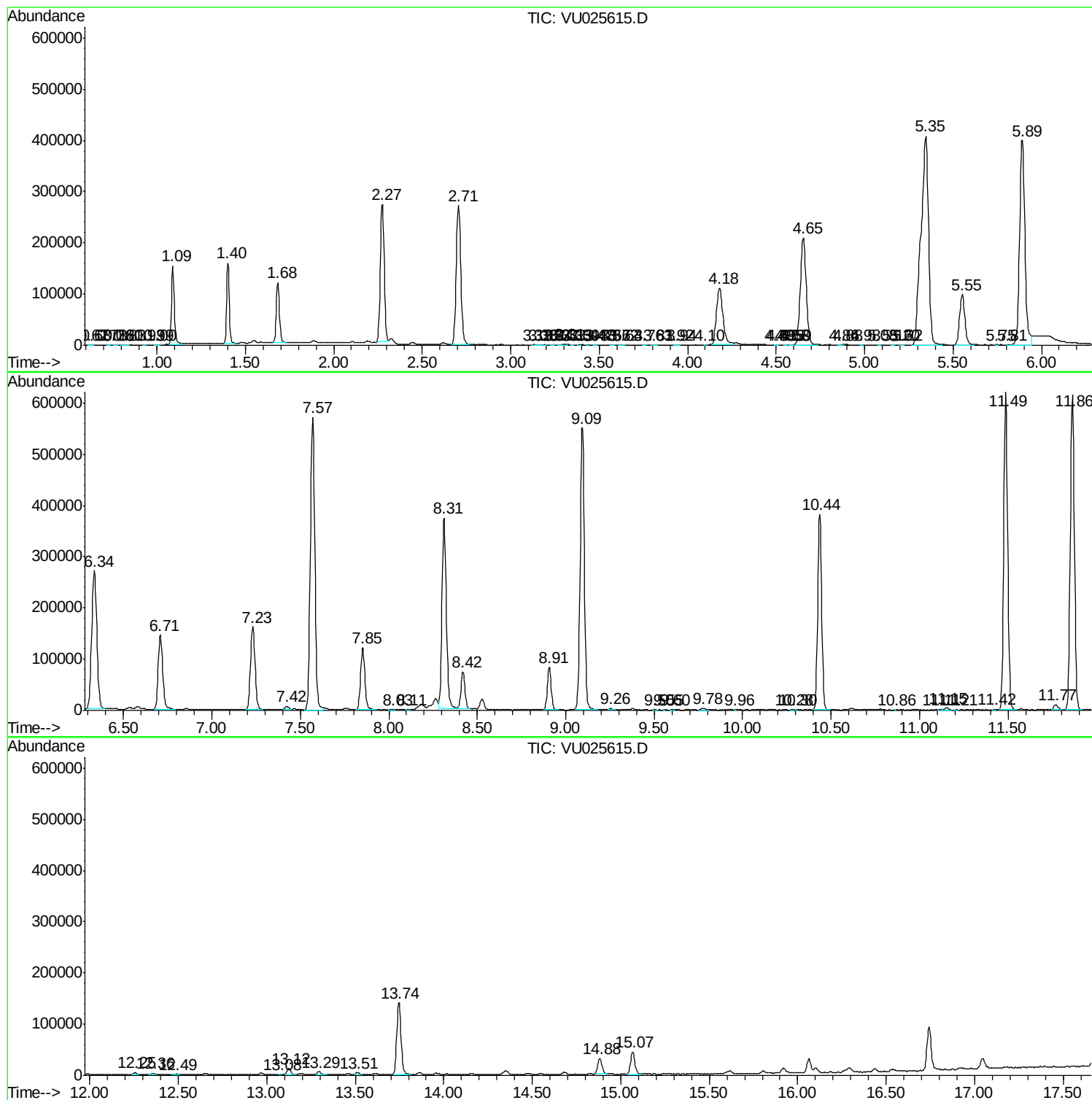
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Instrument :
MSVOA_U
ClientSampled :
VLEB02

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

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



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Instrument :
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ClientSampleId :
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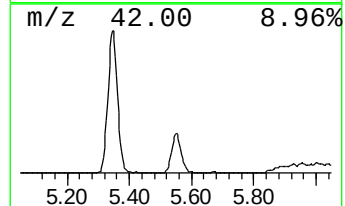
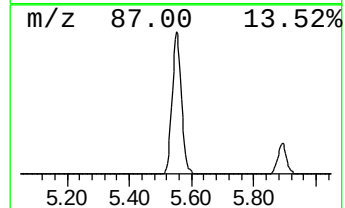
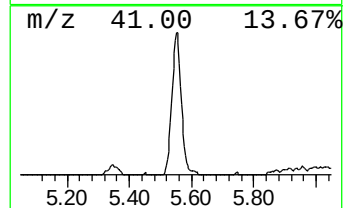
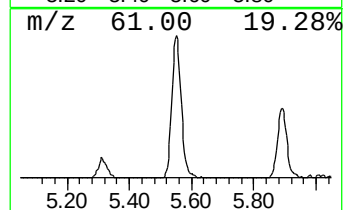
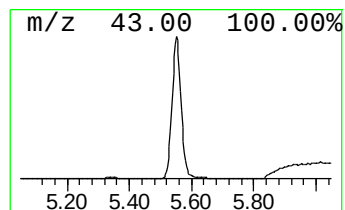
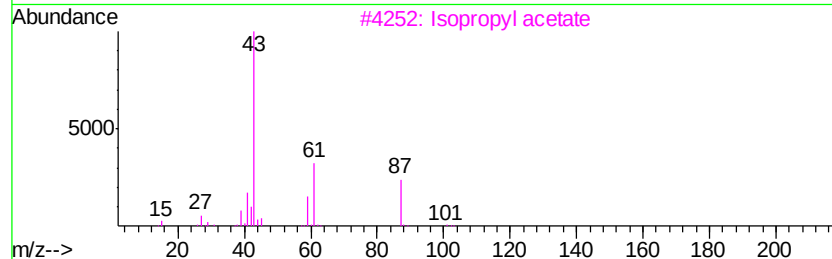
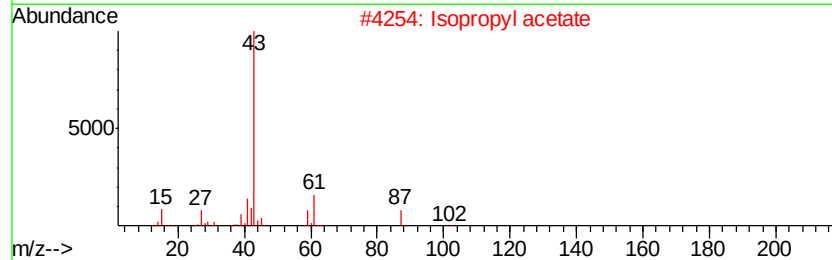
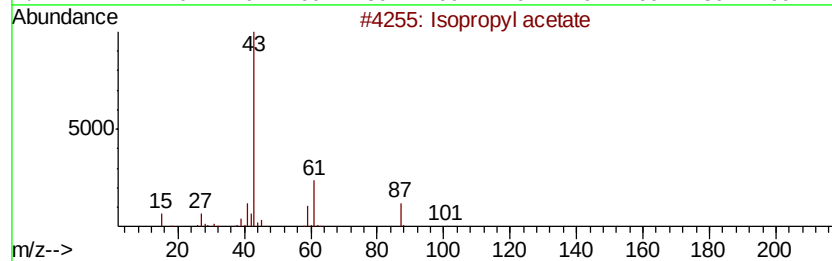
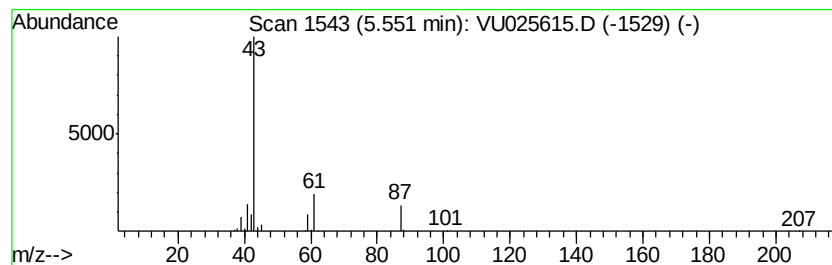
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.55	12.18 ug/L	201391	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	72
3		Isopropyl acetate	102	C5H10O2	000108-21-4	64
4		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	38
5		n-Propyl acetate	102	C5H10O2	000109-60-4	9



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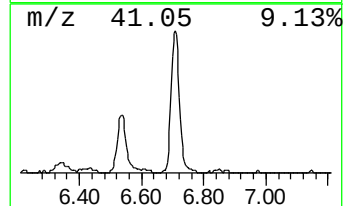
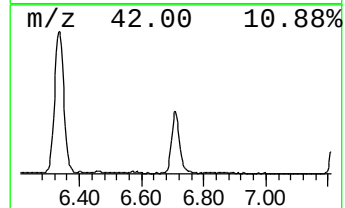
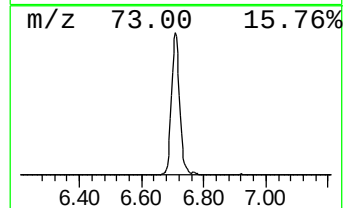
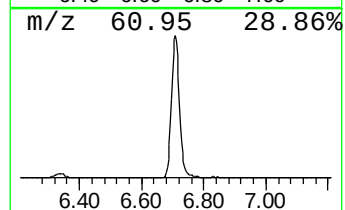
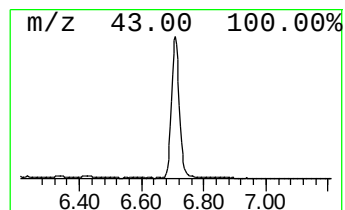
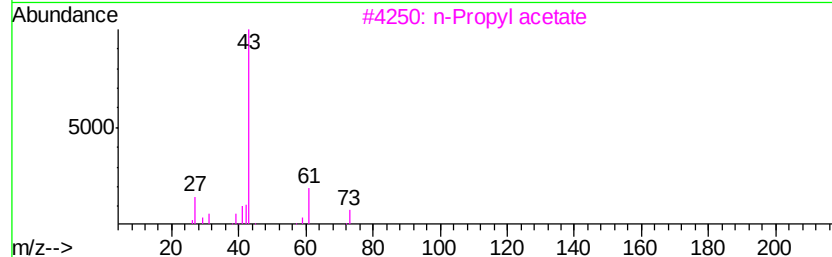
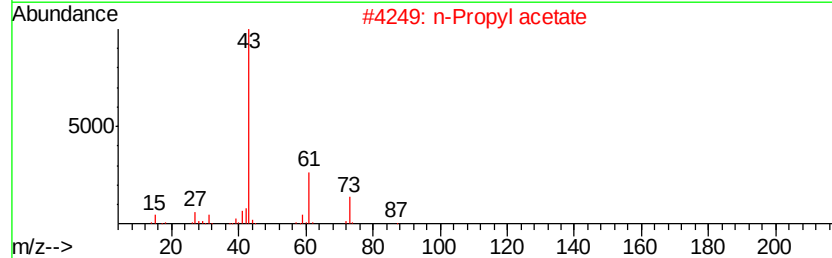
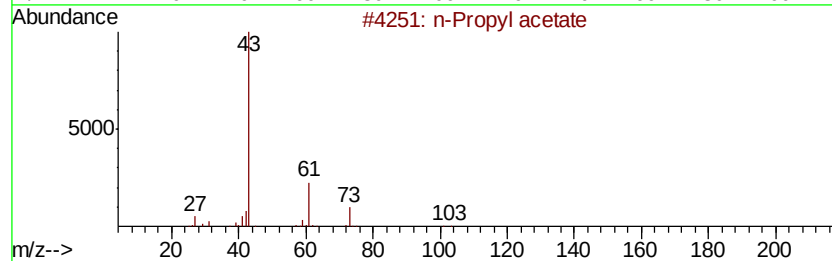
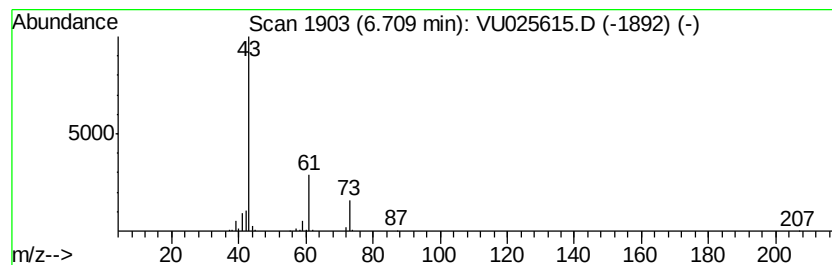
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Quant Title : VOC Analysis

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

Peak Number 3 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	15.74 ug/L	260397	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	83
3		n-Propyl acetate	102	C5H10O2	000109-60-4	64
4		Isopropyl acetate	102	C5H10O2	000108-21-4	9
5		Isobutylamine	73	C4H11N	000078-81-9	7



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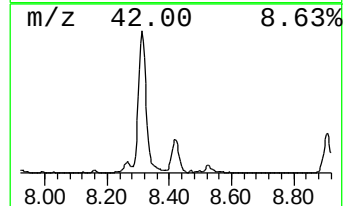
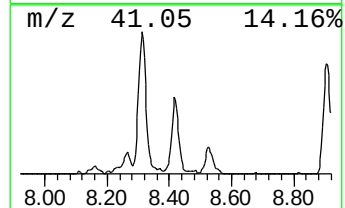
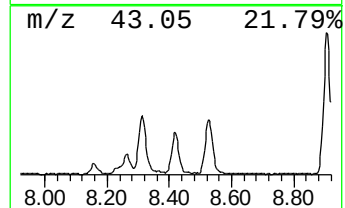
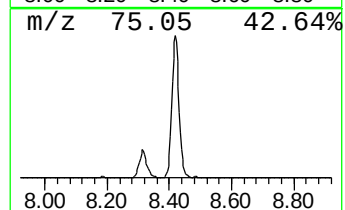
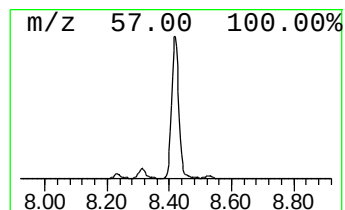
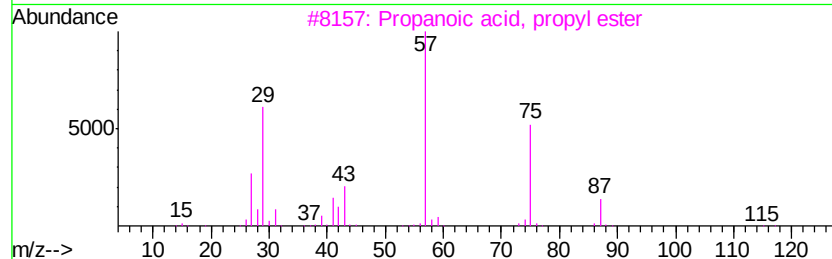
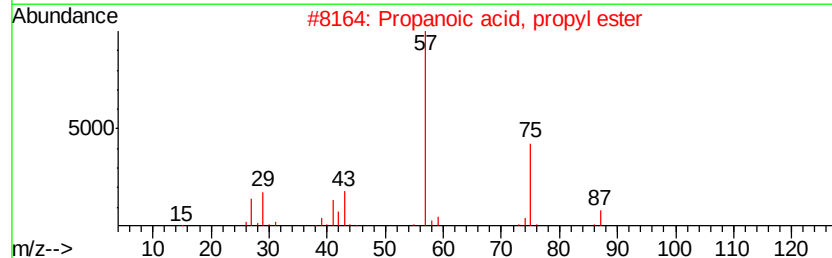
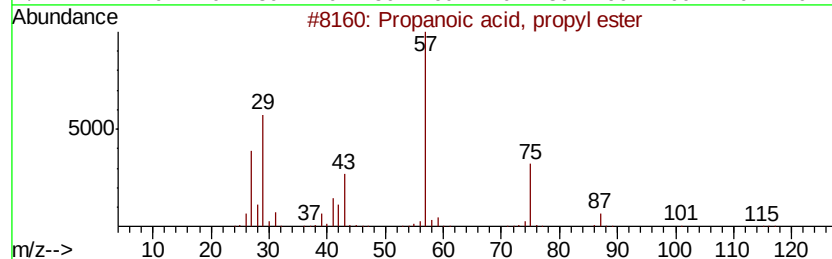
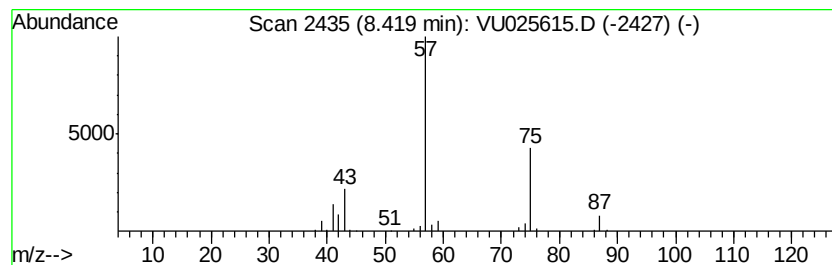
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	6.22 ug/L	113127	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	83
5			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28



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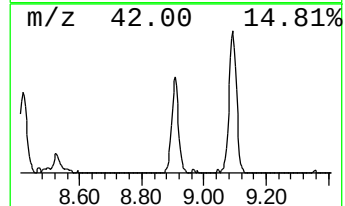
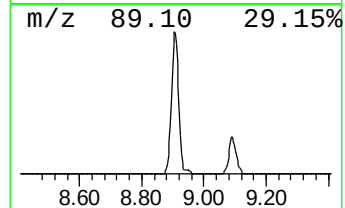
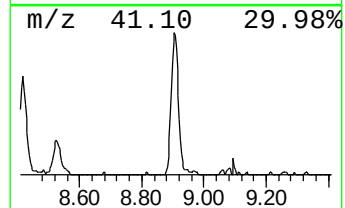
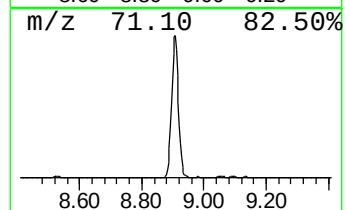
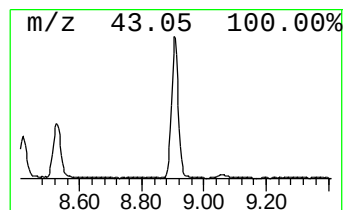
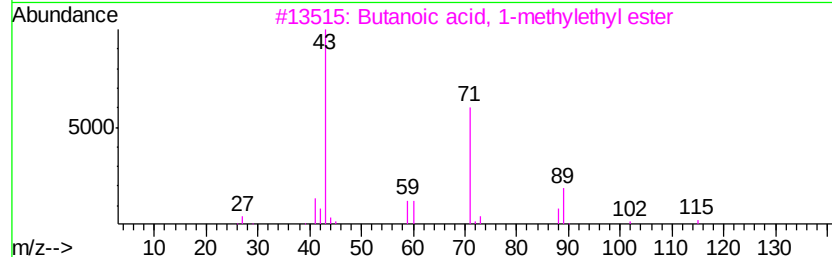
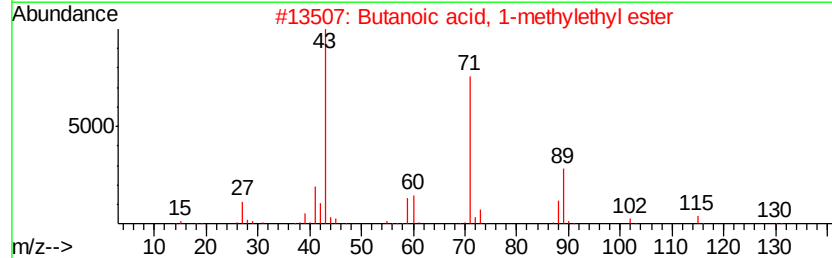
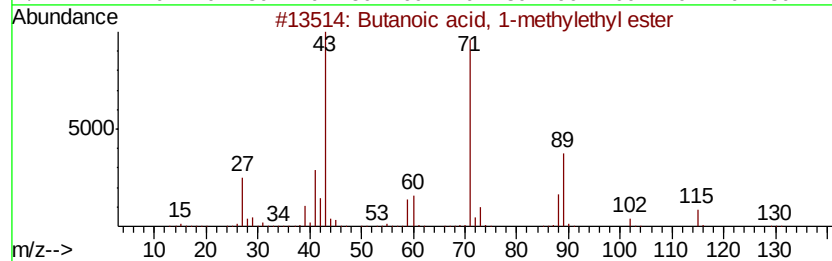
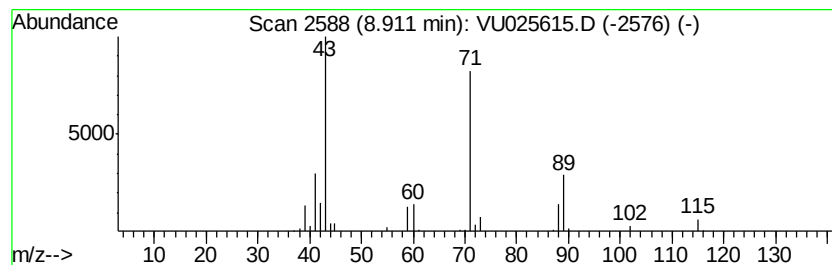
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.91	6.94 ug/L	126333	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	90
4		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5		Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072318\
Data File : VU025615.D
Acq On : 23 Jul 2018 20:38
Operator : MD/SY
Sample : VLEB02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB02

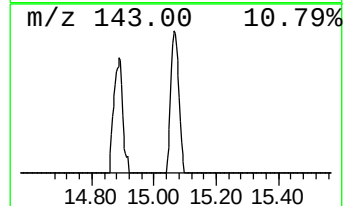
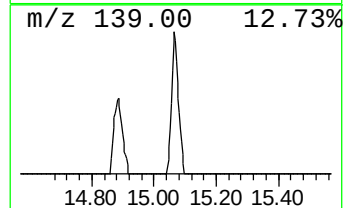
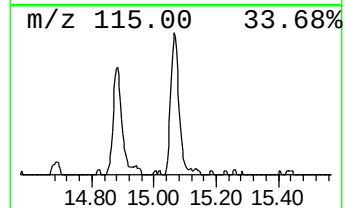
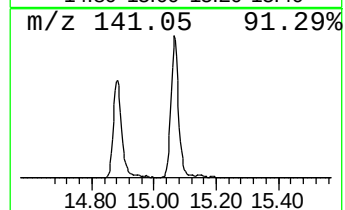
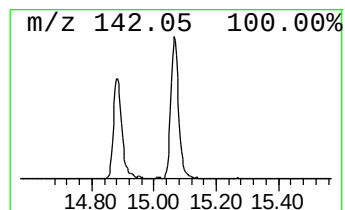
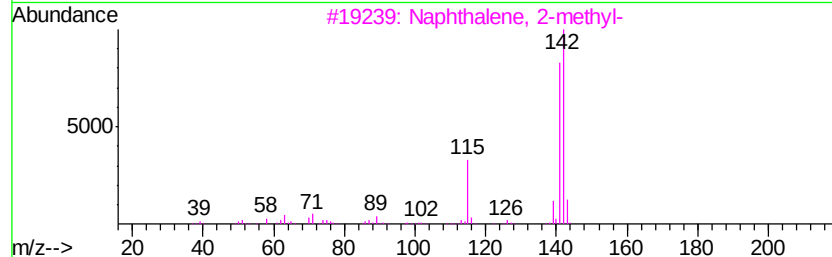
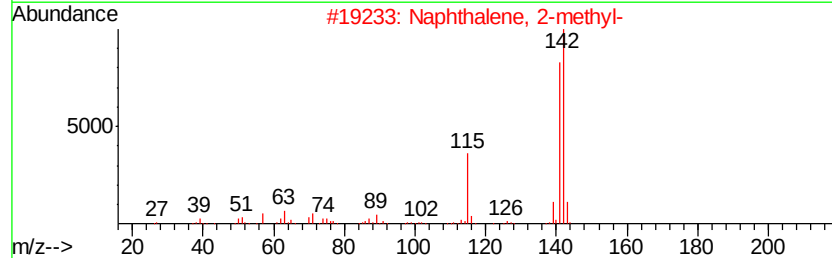
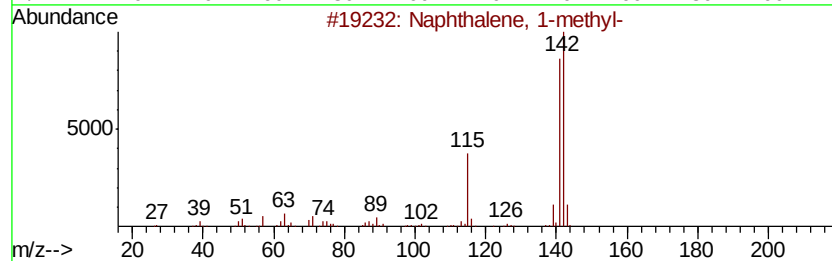
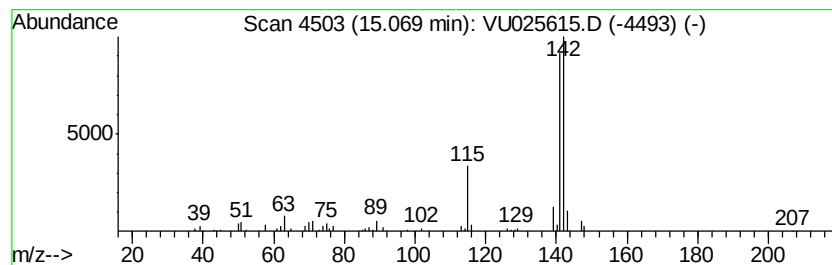
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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	3.87 ug/L	73901	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
4		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	94
5		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072318\
Data File : VU025615.D
Acq On : 23 Jul 2018 20:38
Operator : MD/SY
Sample : VLEB02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB02

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_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	201391	1	5.89	826934	50.0
n-Propyl acetate	6.71	15.7	ug/L	260397	1	5.89	826934	50.0
Propanoic acid, p...	8.42	6.2	ug/L	113127	2	9.09	910051	50.0
Butanoic acid, 1-...	8.91	6.9	ug/L	126333	2	9.09	910051	50.0
Naphthalene, 1-me...	15.07	3.9	ug/L	73901	3	11.49	955474	50.0