

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
 Data File : VV028016.D
 Acq On : 21 Sep 2022 15:06
 Operator : SY/MD
 Sample : N4689-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AY5

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_V\Method\SFAMVLM092022WMA.M

Title : VOC Analysis

Signal : TIC: VV028016.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.298	75	80	99	rVB	181178	194203	14.83%	1.811%
2	1.558	154	161	174	rVB	163390	178961	13.66%	1.669%
3	2.098	319	329	344	rBV	329003	471621	36.01%	4.398%
4	2.741	526	529	530	rBV2	498	234	0.02%	0.002%
5	2.844	558	561	563	rBV2	639	368	0.03%	0.003%
6	2.970	594	600	602	rBV4	742	739	0.06%	0.007%
7	3.098	638	640	642	rBV	459	246	0.02%	0.002%
8	3.114	642	645	649	rVB3	874	481	0.04%	0.004%
9	3.172	655	663	667	rBV4	2162	2875	0.22%	0.027%
10	3.320	707	709	713	rVB3	625	371	0.03%	0.003%
11	3.394	729	732	735	rVB3	562	302	0.02%	0.003%
12	3.642	805	809	810	rBV2	489	265	0.02%	0.002%
13	3.873	870	881	922	rBV2	124749	368503	28.14%	3.437%
14	4.339	1010	1026	1057	rBV	232164	566843	43.28%	5.286%
15	4.671	1126	1129	1133	rBV4	826	733	0.06%	0.007%
16	4.722	1142	1145	1148	rBV3	536	294	0.02%	0.003%
17	4.751	1152	1154	1155	rBV	477	222	0.02%	0.002%
18	4.822	1174	1176	1180	rBV3	528	315	0.02%	0.003%
19	4.883	1193	1195	1199	rVB2	548	297	0.02%	0.003%
20	5.037	1223	1243	1277	rBV2	505281	1309723	100.00%	12.214%
21	5.214	1296	1298	1299	rBV2	517	274	0.02%	0.003%
22	5.285	1311	1320	1337	rBV4	6962	17322	1.32%	0.162%
23	5.436	1365	1367	1370	rBV3	442	327	0.02%	0.003%
24	5.609	1410	1421	1443	rBV	414339	895757	68.39%	8.354%
25	6.063	1551	1562	1587	rVB	325484	656999	50.16%	6.127%
26	6.458	1677	1685	1716	rBV	113051	222413	16.98%	2.074%
27	6.982	1837	1848	1866	rBV	169339	311511	23.78%	2.905%
28	7.185	1903	1911	1924	rBV	19325	32052	2.45%	0.299%
29	7.310	1938	1950	1968	rBV	558793	968764	73.97%	9.035%
30	7.616	2035	2045	2069	rBV2	131855	239899	18.32%	2.237%
31	7.844	2111	2116	2120	rBV4	945	757	0.06%	0.007%
32	7.924	2132	2141	2161	rVB2	25667	46048	3.52%	0.429%
33	8.085	2181	2191	2216	rBV	410521	714514	54.55%	6.664%
34	8.304	2251	2259	2274	rVB2	26955	47189	3.60%	0.440%
35	8.680	2365	2376	2391	rBV	82490	136069	10.39%	1.269%
36	8.847	2417	2428	2450	rBV	574914	937243	71.56%	8.741%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
 Data File : VV028016.D
 Acq On : 21 Sep 2022 15:06
 Operator : SY/MD
 Sample : N4689-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AY5

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_V\Method\SFAMVLM092022WMA.M
 Title : VOC Analysis

37	9.182	2530	2532	2535	rBV	414	255	0.02%	0.002%
38	9.214	2540	2542	2547	rVB2	745	458	0.03%	0.004%
39	9.278	2556	2562	2564	rBV3	532	548	0.04%	0.005%
40	9.323	2574	2576	2579	rVB2	645	297	0.02%	0.003%
41	9.342	2579	2582	2587	rVB4	820	822	0.06%	0.008%
42	9.391	2590	2597	2600	rBV4	1080	1206	0.09%	0.011%
43	9.551	2637	2647	2656	rBV4	6513	11288	0.86%	0.105%
44	9.661	2676	2681	2686	rBV5	692	886	0.07%	0.008%
45	9.928	2755	2764	2765	rBV2	488	518	0.04%	0.005%
46	9.985	2778	2782	2784	rBV2	379	223	0.02%	0.002%
47	10.014	2787	2791	2794	rBV	510	451	0.03%	0.004%
48	10.034	2794	2797	2800	rVB	469	323	0.02%	0.003%
49	10.127	2817	2826	2834	rVB8	1312	2228	0.17%	0.021%
50	10.159	2834	2836	2839	rBV4	465	252	0.02%	0.002%
51	10.211	2839	2852	2873	rBV	424700	665280	50.80%	6.204%
52	10.355	2895	2897	2899	rBV4	648	322	0.02%	0.003%
53	10.481	2933	2936	2939	rVB2	541	278	0.02%	0.003%
54	10.603	2970	2974	2975	rBV2	361	239	0.02%	0.002%
55	10.767	3021	3025	3026	rBV	329	232	0.02%	0.002%
56	10.911	3061	3070	3072	rBV5	1140	1369	0.10%	0.013%
57	10.979	3089	3091	3094	rBV3	378	236	0.02%	0.002%
58	10.998	3094	3097	3099	rBV2	313	218	0.02%	0.002%
59	11.027	3104	3106	3113	rVB3	645	619	0.05%	0.006%
60	11.079	3117	3122	3123	rBV2	426	321	0.02%	0.003%
61	11.146	3139	3143	3147	rBV3	1017	897	0.07%	0.008%
62	11.246	3163	3174	3194	rBV	539720	822160	62.77%	7.667%
63	11.474	3239	3245	3249	rBV3	617	757	0.06%	0.007%
64	11.526	3259	3261	3264	rVB	416	265	0.02%	0.002%
65	11.622	3278	3291	3310	rBV	549431	870711	66.48%	8.120%
66	11.821	3351	3353	3357	rBV4	509	247	0.02%	0.002%
67	11.844	3357	3360	3364	rVV4	865	612	0.05%	0.006%
68	11.863	3364	3366	3369	rVB2	515	279	0.02%	0.003%
69	11.895	3372	3376	3381	rBV4	500	563	0.04%	0.005%
70	11.966	3391	3398	3401	rBV4	459	649	0.05%	0.006%
71	12.046	3420	3423	3426	rBV2	401	233	0.02%	0.002%
72	12.120	3443	3446	3452	rBV2	375	391	0.03%	0.004%
73	12.178	3462	3464	3467	rBV3	398	224	0.02%	0.002%
74	12.239	3480	3483	3490	rVV4	606	662	0.05%	0.006%
75	12.284	3493	3497	3500	rVB	340	223	0.02%	0.002%
76	12.307	3500	3504	3506	rBV3	384	218	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
 Data File : VV028016.D
 Acq On : 21 Sep 2022 15:06
 Operator : SY/MD
 Sample : N4689-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AY5

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_V\Method\SFAMVLM092022WMA.M
 Title : VOC Analysis

77	12.397	3528	3532	3536	rVB3	633	480	0.04%	0.004%
78	12.481	3557	3558	3564	rVB3	343	249	0.02%	0.002%
79	12.529	3571	3573	3578	rVB2	331	242	0.02%	0.002%
80	12.780	3648	3651	3654	rBV2	489	301	0.02%	0.003%
81	12.802	3654	3658	3663	rVV4	812	695	0.05%	0.006%
82	12.825	3663	3665	3667	rVB	553	222	0.02%	0.002%
83	12.873	3678	3680	3682	rBV	432	215	0.02%	0.002%
84	13.185	3773	3777	3780	rBV	368	272	0.02%	0.003%
85	13.210	3780	3785	3788	rBV3	528	446	0.03%	0.004%
86	13.381	3835	3838	3842	rVB3	332	260	0.02%	0.002%
87	13.407	3842	3846	3850	rBV3	703	434	0.03%	0.004%
88	13.432	3851	3854	3856	rBV2	426	233	0.02%	0.002%
89	13.529	3883	3884	3889	rVB2	665	295	0.02%	0.003%
90	13.712	3938	3941	3943	rBV2	318	231	0.02%	0.002%
91	13.754	3950	3954	3955	rBV	482	300	0.02%	0.003%
92	13.837	3976	3980	3984	rBV4	471	466	0.04%	0.004%
93	13.876	3989	3992	3997	rVB3	822	560	0.04%	0.005%
94	13.902	3997	4000	4003	rBV	437	357	0.03%	0.003%
95	14.316	4127	4129	4132	rVB3	696	313	0.02%	0.003%
96	14.416	4153	4160	4163	rBV5	613	799	0.06%	0.007%
97	14.503	4185	4187	4191	rBV3	627	357	0.03%	0.003%
98	14.574	4205	4209	4215	rBV7	936	1094	0.08%	0.010%
99	14.792	4272	4277	4281	rBV2	810	875	0.07%	0.008%
100	14.866	4296	4300	4301	rBV2	465	365	0.03%	0.003%

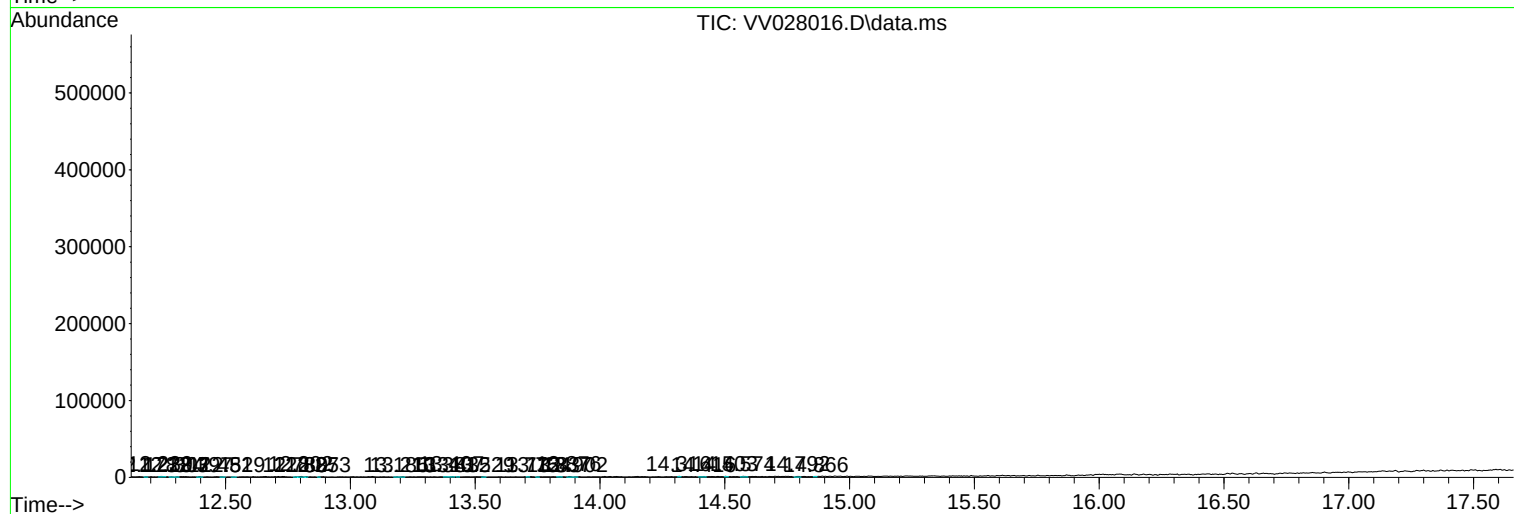
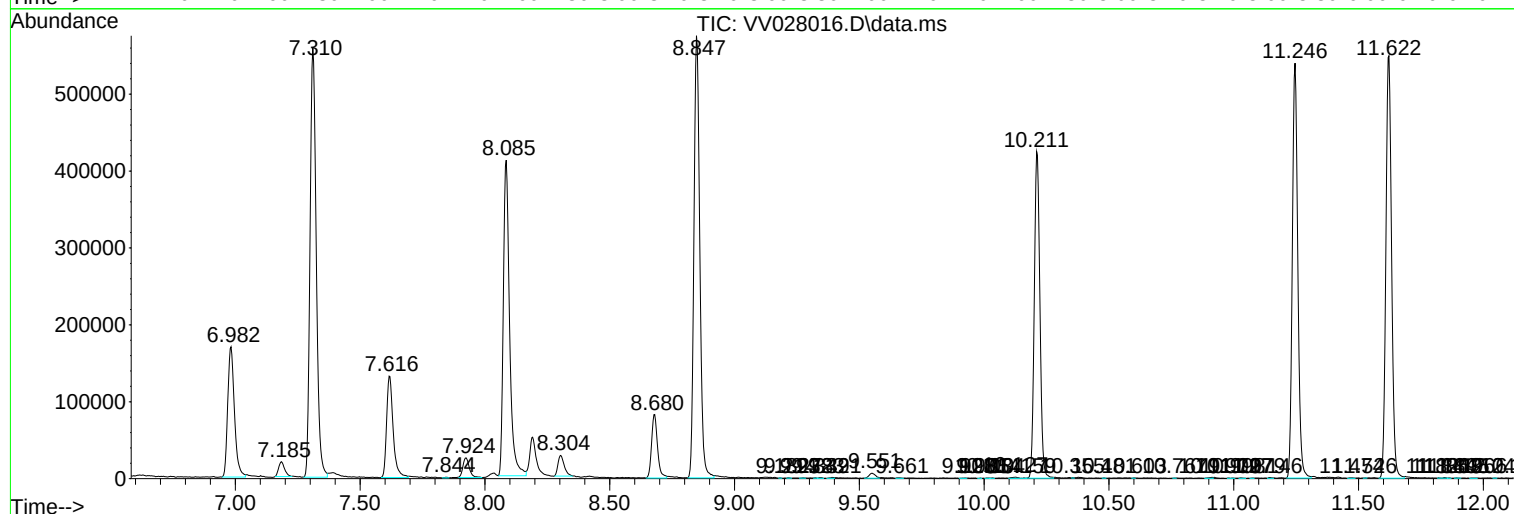
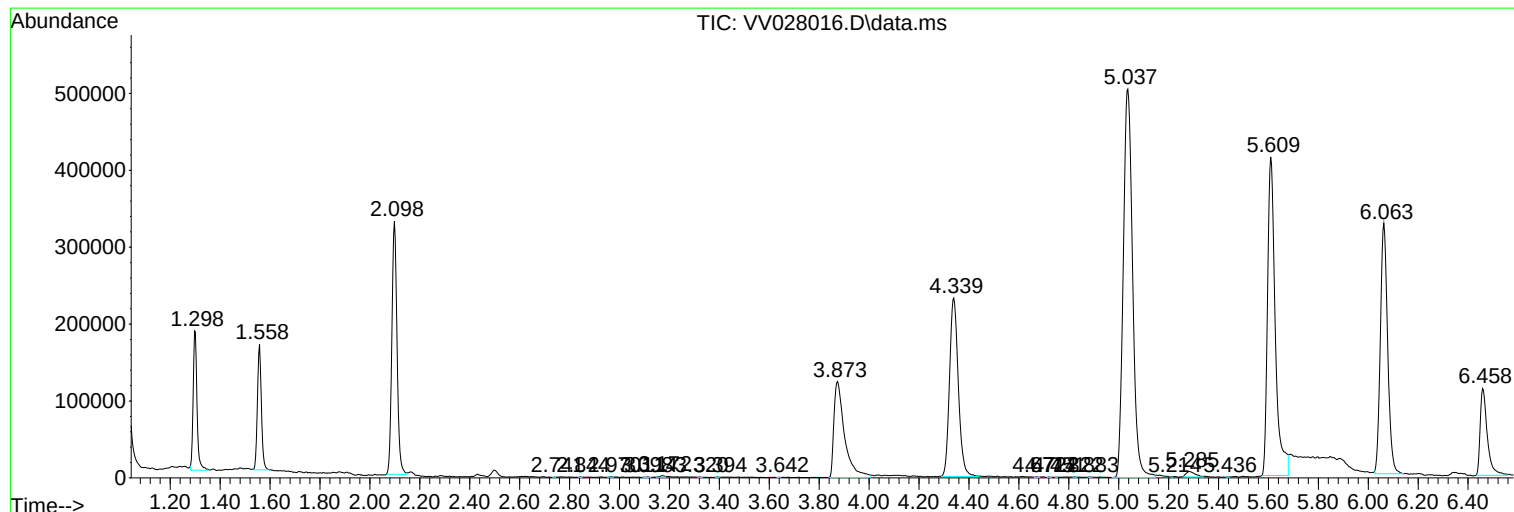
Sum of corrected areas: 10722755

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028016.D
Acq On : 21 Sep 2022 15:06
Operator : SY/MD
Sample : N4689-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028016.D
Acq On : 21 Sep 2022 15:06
Operator : SY/MD
Sample : N4689-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY5

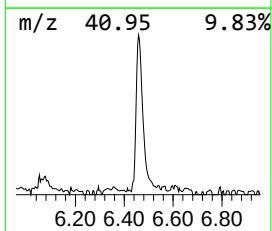
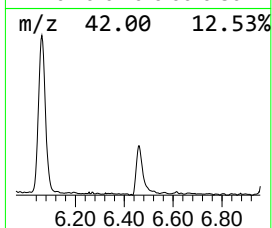
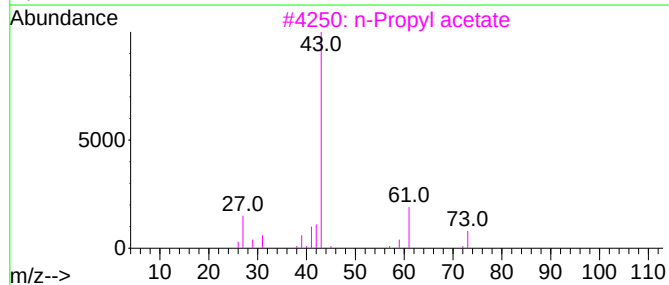
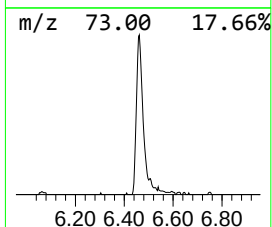
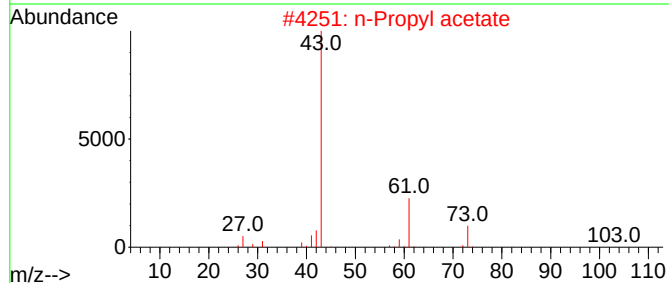
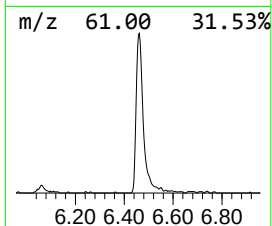
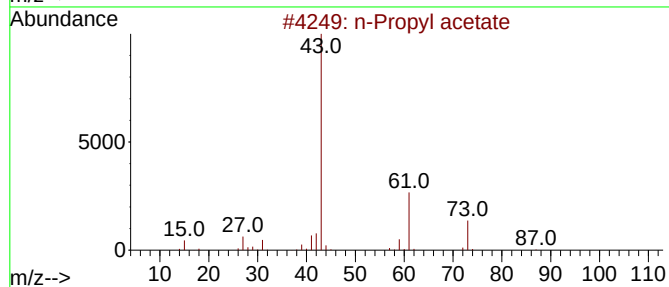
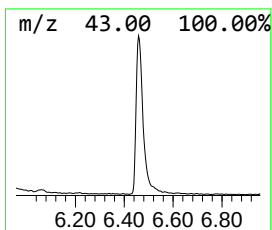
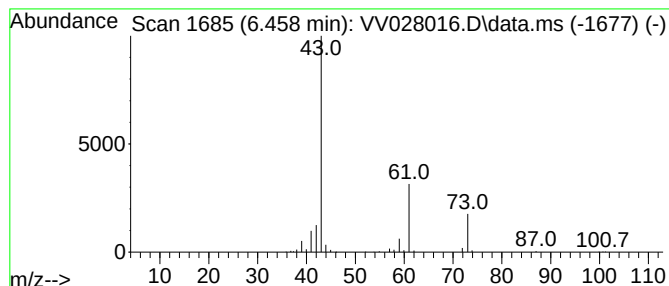
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.458	12.41 ug/L	222413	1,4-Difluorobenzene	5.609

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	72
3	n-Propyl acetate			102	C5H10O2	000109-60-4	56
4	Isopropyl acetate			102	C5H10O2	000108-21-4	36
5	Propanal, 2,3-dihydroxy-, (S)-			90	C3H6O3	000497-09-6	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028016.D
Acq On : 21 Sep 2022 15:06
Operator : SY/MD
Sample : N4689-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY5

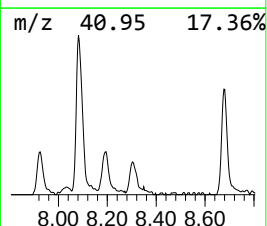
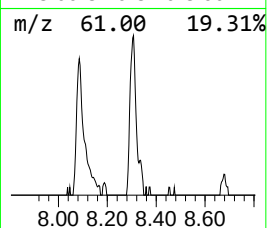
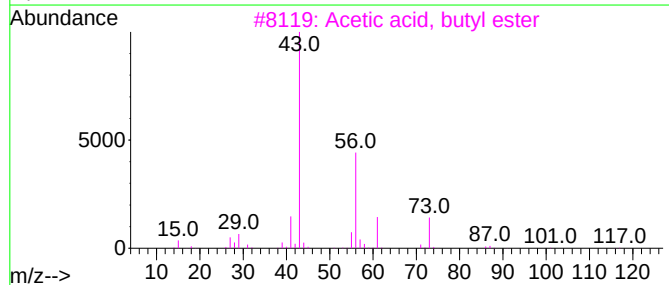
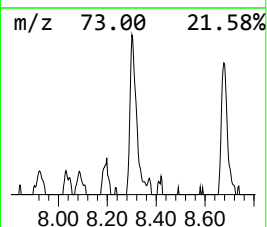
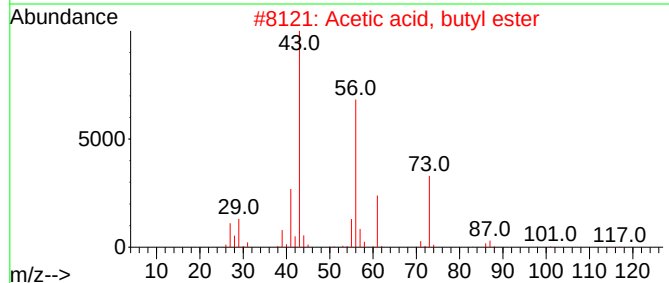
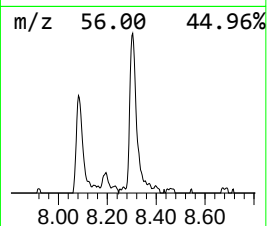
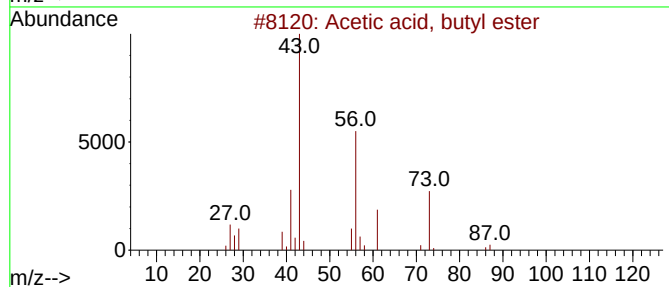
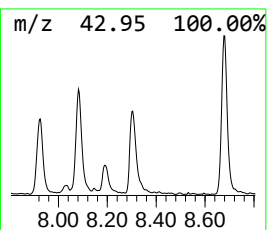
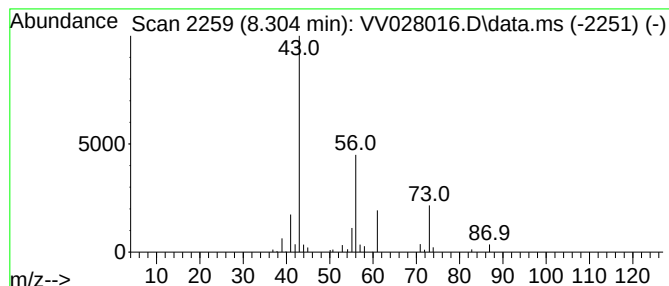
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.304	2.52 ug/L	47189	Chlorobenzene-d5	8.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	59
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
4			Isobutyl acetate	116	C6H12O2	000110-19-0	45
5			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028016.D
Acq On : 21 Sep 2022 15:06
Operator : SY/MD
Sample : N4689-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY5

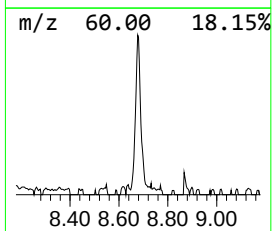
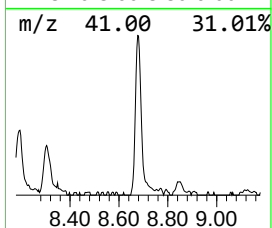
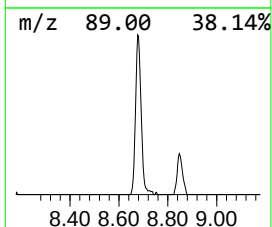
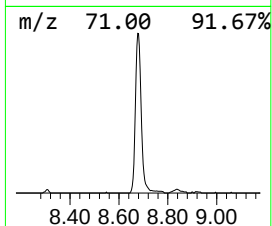
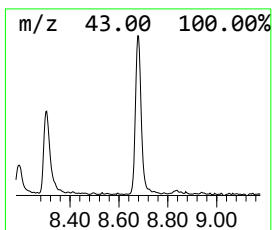
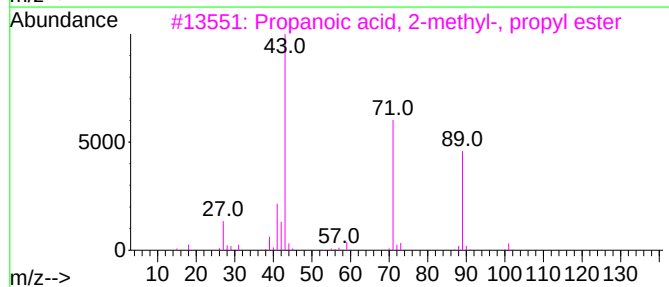
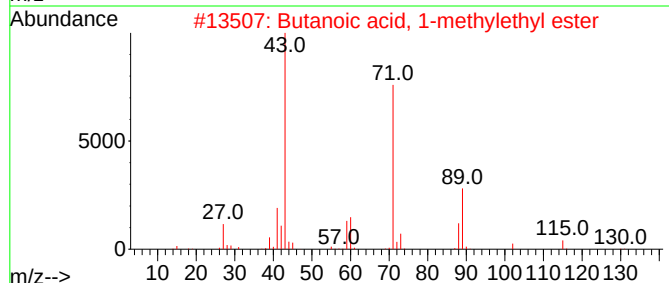
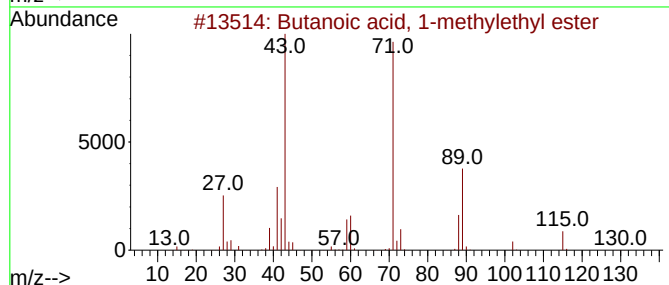
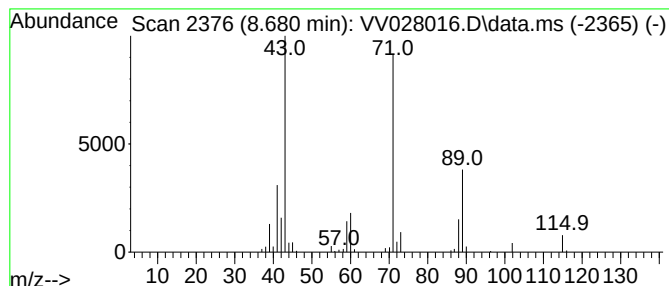
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.680	7.26 ug/L	136069	Chlorobenzene-d5	8.847

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			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
5			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028016.D
Acq On : 21 Sep 2022 15:06
Operator : SY/MD
Sample : N4689-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.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	6.458	12.4	ug/L	222413	1	5.609	895757	50.0
Acetic acid, bu...	8.304	2.5	ug/L	47189	2	8.847	937243	50.0
Butanoic acid, ...	8.680	7.3	ug/L	136069	2	8.847	937243	50.0