

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
 Data File : VV020301.D
 Acq On : 11 Feb 2021 16:29
 Operator : SY/MD
 Sample : PB134573TB
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB01

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\SOMVLM020521WMA.M

Title : VOC Analysis

Signal : TIC: VV020301.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	76	83	98	rVB	270308	277316	5.28%	0.929%
2	1.568	157	164	180	rVB	239142	270851	5.15%	0.907%
3	2.111	322	333	348	rBV	482009	730862	13.90%	2.448%
4	2.510	448	457	472	rBV2	16320	27916	0.53%	0.094%
5	2.584	477	480	482	rBV3	590	460	0.01%	0.002%
6	2.664	501	505	506	rBV2	747	554	0.01%	0.002%
7	2.767	535	537	541	rVB2	645	369	0.01%	0.001%
8	2.934	586	589	590	rBV2	611	388	0.01%	0.001%
9	3.069	626	631	635	rVB6	712	626	0.01%	0.002%
10	3.095	635	639	642	rBV2	637	499	0.01%	0.002%
11	3.121	642	647	654	rVB3	623	561	0.01%	0.002%
12	3.178	654	665	683	rBV7	4189	11595	0.22%	0.039%
13	3.680	818	821	824	rVV2	795	587	0.01%	0.002%
14	3.699	824	827	828	rVV3	577	339	0.01%	0.001%
15	3.712	829	831	839	rVB5	834	607	0.01%	0.002%
16	3.841	864	871	874	rBV3	672	810	0.02%	0.003%
17	3.883	874	884	919	rBV	145065	422911	8.04%	1.417%
18	4.275	1004	1006	1009	rVB4	572	338	0.01%	0.001%
19	4.352	1009	1030	1060	rBV	298776	788857	15.01%	2.643%
20	4.522	1080	1083	1085	rBV2	532	321	0.01%	0.001%
21	4.838	1178	1181	1186	rBV2	544	547	0.01%	0.002%
22	5.050	1229	1247	1275	rBV2	762707	1960411	37.29%	6.567%
23	5.288	1310	1321	1340	rBV3	21553	50734	0.97%	0.170%
24	5.394	1349	1354	1357	rBV4	528	491	0.01%	0.002%
25	5.484	1380	1382	1385	rBV	747	614	0.01%	0.002%
26	5.538	1396	1399	1401	rVV3	533	416	0.01%	0.001%
27	5.619	1411	1424	1447	rBV	700101	1425440	27.12%	4.775%
28	6.072	1552	1565	1591	rVB	437158	886917	16.87%	2.971%
29	6.194	1595	1603	1614	rBV3	9367	19582	0.37%	0.066%
30	6.345	1633	1650	1652	rBV2	18543	33206	0.63%	0.111%
31	6.461	1674	1686	1722	rBV	1905768	3312275	63.01%	11.095%
32	6.989	1839	1850	1871	rBV	247245	444681	8.46%	1.490%
33	7.188	1900	1912	1924	rBV	288216	491651	9.35%	1.647%
34	7.320	1941	1953	1978	rBV	939045	1626226	30.93%	5.448%
35	7.558	2022	2027	2035	rBV6	3315	4686	0.09%	0.016%
36	7.625	2037	2048	2069	rBV2	195731	343625	6.54%	1.151%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
 Title : VOC Analysis

37	7.927	2131	2142	2156	rBV	80960	138416	2.63%	0.464%
38	8.037	2163	2176	2184	rBV	204271	320526	6.10%	1.074%
39	8.091	2184	2193	2213	rVV	593407	1024929	19.50%	3.433%
40	8.191	2213	2224	2249	rVV	3478470	5256921	100.00%	17.610%
41	8.304	2250	2259	2284	rVB	320495	522437	9.94%	1.750%
42	8.683	2365	2377	2408	rBV	2160595	3215647	61.17%	10.772%
43	8.857	2418	2431	2459	rBV	1125766	1812219	34.47%	6.071%
44	9.342	2578	2582	2583	rBV2	643	384	0.01%	0.001%
45	9.397	2594	2599	2606	rBV4	2579	3111	0.06%	0.010%
46	9.551	2638	2647	2668	rBV2	63196	102309	1.95%	0.343%
47	9.673	2681	2685	2690	rBV5	665	786	0.01%	0.003%
48	9.760	2709	2712	2714	rBV3	1105	797	0.02%	0.003%
49	9.857	2738	2742	2745	rBV3	719	752	0.01%	0.003%
50	10.017	2789	2792	2798	rBV4	536	561	0.01%	0.002%
51	10.114	2818	2822	2825	rBV3	539	505	0.01%	0.002%
52	10.162	2834	2837	2840	rBV3	388	339	0.01%	0.001%
53	10.223	2843	2856	2878	rBV	620945	964124	18.34%	3.230%
54	10.493	2937	2940	2942	rBV4	648	330	0.01%	0.001%
55	10.513	2944	2946	2948	rVV3	616	329	0.01%	0.001%
56	10.545	2948	2956	2966	rVV3	13611	21126	0.40%	0.071%
57	10.622	2977	2980	2985	rVB5	817	721	0.01%	0.002%
58	10.654	2986	2990	2995	rVB3	679	620	0.01%	0.002%
59	10.680	2995	2998	3001	rBV3	618	453	0.01%	0.002%
60	10.834	3042	3046	3047	rBV	524	367	0.01%	0.001%
61	10.921	3070	3073	3074	rBV2	725	424	0.01%	0.001%
62	10.969	3085	3088	3093	rBV5	511	511	0.01%	0.002%
63	10.995	3093	3096	3099	rBV4	463	405	0.01%	0.001%
64	11.104	3124	3130	3133	rBV6	715	685	0.01%	0.002%
65	11.255	3164	3177	3200	rBV	1133723	1749609	33.28%	5.861%
66	11.455	3237	3239	3243	rVB4	723	409	0.01%	0.001%
67	11.538	3262	3265	3273	rBV5	876	1236	0.02%	0.004%
68	11.631	3279	3294	3312	rBV	994936	1554255	29.57%	5.206%
69	11.821	3349	3353	3356	rBV3	896	700	0.01%	0.002%
70	11.844	3357	3360	3364	rVB4	742	618	0.01%	0.002%
71	11.876	3366	3370	3372	rBV4	513	398	0.01%	0.001%
72	11.918	3380	3383	3386	rBV2	513	481	0.01%	0.002%
73	12.139	3447	3452	3453	rBV3	583	516	0.01%	0.002%
74	12.165	3457	3460	3464	rBV3	357	355	0.01%	0.001%
75	12.262	3488	3490	3496	rVB3	839	671	0.01%	0.002%
76	12.316	3502	3507	3510	rBV2	609	588	0.01%	0.002%

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Title : VOC Analysis

77	12.352	3516	3518	3520	rBV2	643	376	0.01%	0.001%
78	12.371	3522	3524	3531	rVB6	821	520	0.01%	0.002%
79	12.644	3606	3609	3614	rVV5	737	719	0.01%	0.002%
80	12.725	3630	3634	3636	rBV3	893	666	0.01%	0.002%
81	12.773	3647	3649	3654	rVB4	560	383	0.01%	0.001%
82	12.879	3680	3682	3686	rVB3	715	427	0.01%	0.001%
83	12.902	3686	3689	3693	rBV2	531	398	0.01%	0.001%
84	12.930	3695	3698	3703	rBV5	661	531	0.01%	0.002%
85	13.130	3757	3760	3766	rVB4	606	541	0.01%	0.002%
86	13.159	3766	3769	3774	rVB4	596	551	0.01%	0.002%
87	13.188	3774	3778	3780	rBV5	453	407	0.01%	0.001%
88	13.197	3780	3781	3785	rVB3	680	337	0.01%	0.001%
89	13.274	3802	3805	3807	rBV2	861	418	0.01%	0.001%
90	13.377	3831	3837	3838	rBV3	585	546	0.01%	0.002%
91	13.522	3876	3882	3884	rBV4	1053	1158	0.02%	0.004%
92	13.570	3894	3897	3902	rBV4	742	499	0.01%	0.002%
93	13.673	3924	3929	3934	rBV4	868	1077	0.02%	0.004%
94	13.750	3951	3953	3956	rVB3	814	487	0.01%	0.002%
95	13.901	3996	4000	4001	rBV3	462	342	0.01%	0.001%
96	13.988	4022	4027	4030	rBV2	853	914	0.02%	0.003%
97	14.210	4094	4096	4101	rVB4	767	554	0.01%	0.002%
98	14.715	4250	4253	4256	rVV3	739	456	0.01%	0.002%
99	14.937	4319	4322	4325	rBV3	748	619	0.01%	0.002%
100	15.210	4403	4407	4410	rBV5	692	691	0.01%	0.002%

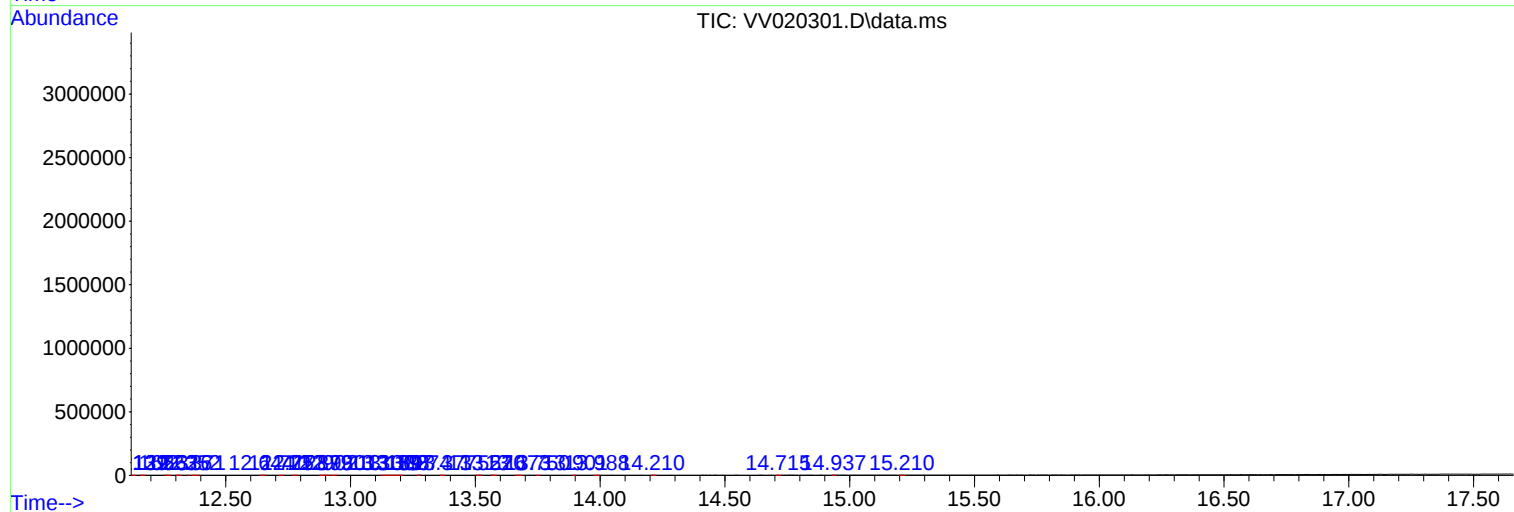
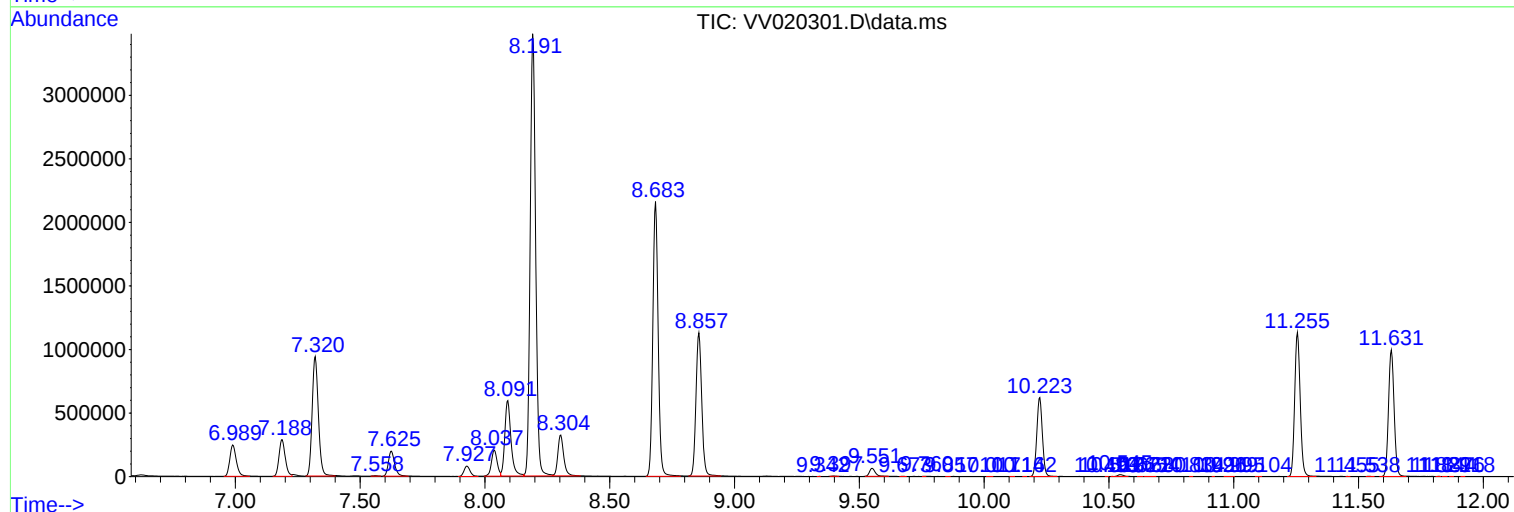
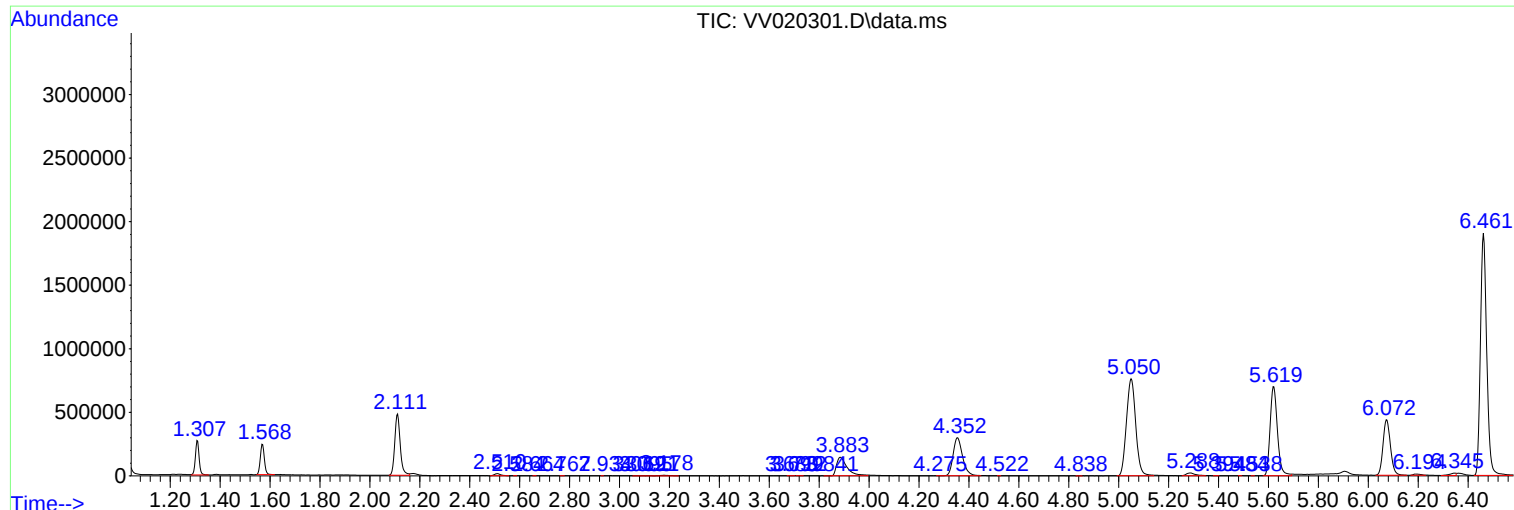
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Instrument :
MSVOA_V
ClientSampleId :
VLEB01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

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



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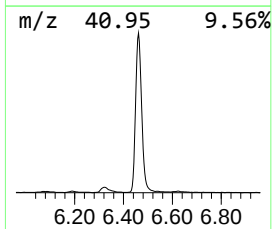
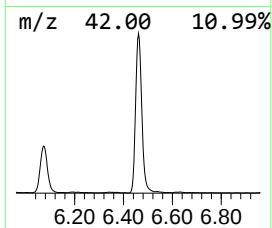
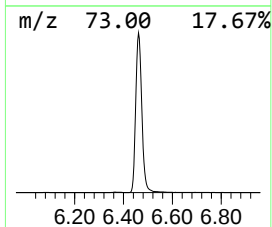
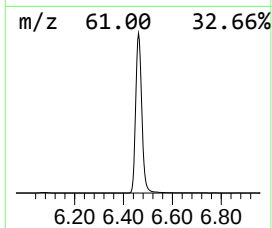
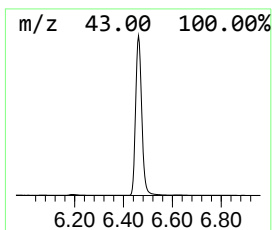
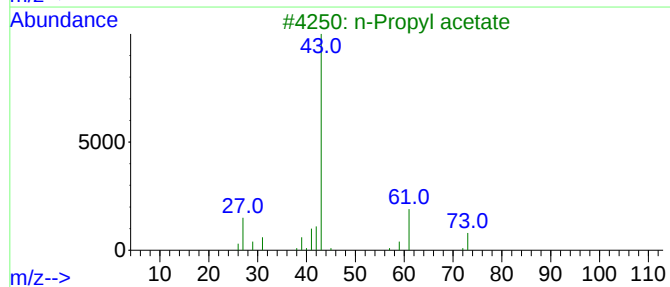
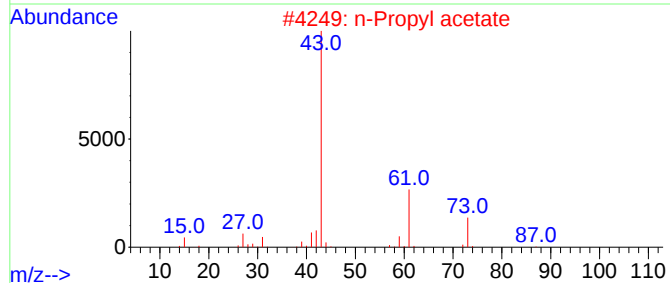
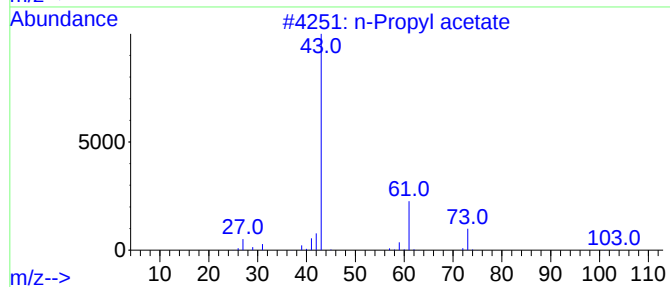
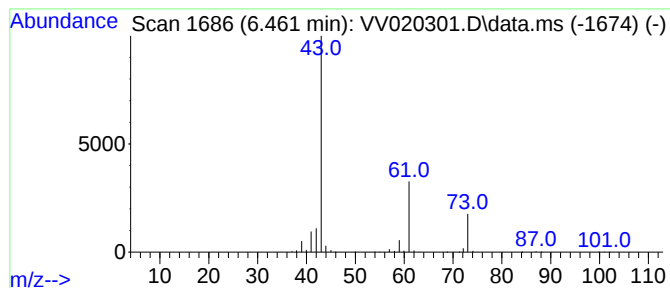
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

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.
6.461	116.18 ug/L	3312280	1,4-Difluorobenzene	5.619

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	83
3	n-Propyl acetate			102	C5H10O2	000109-60-4	78
4	Propanal, 2,3-dihydroxy-, (S)-			90	C3H6O3	000497-09-6	36
5	Isopropyl acetate			102	C5H10O2	000108-21-4	36



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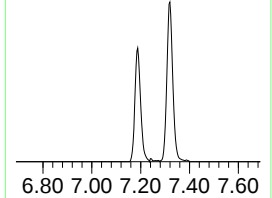
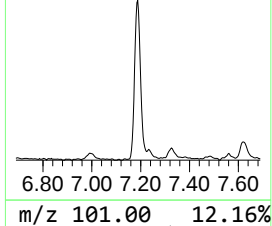
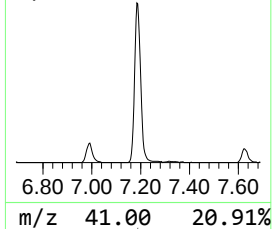
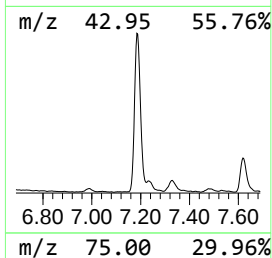
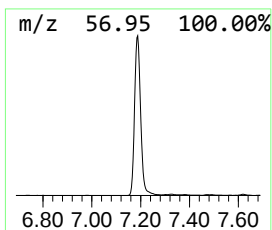
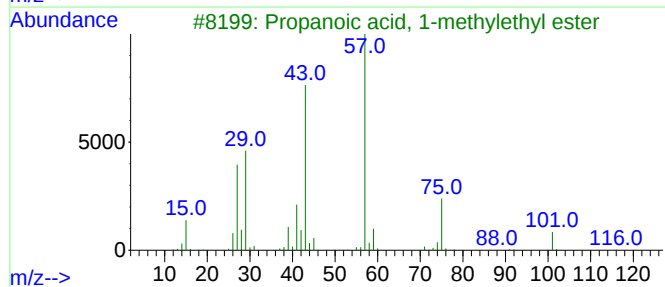
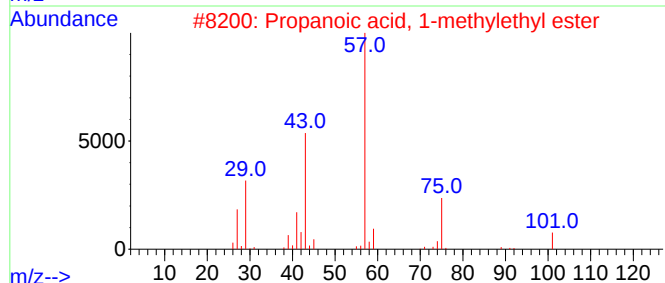
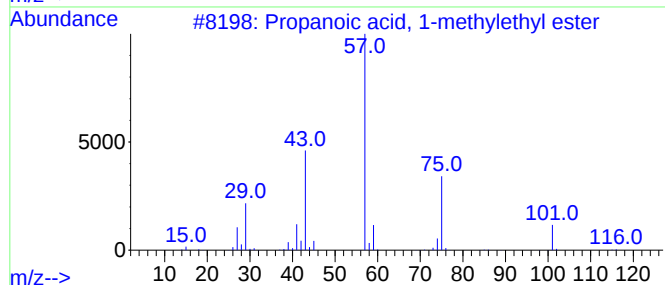
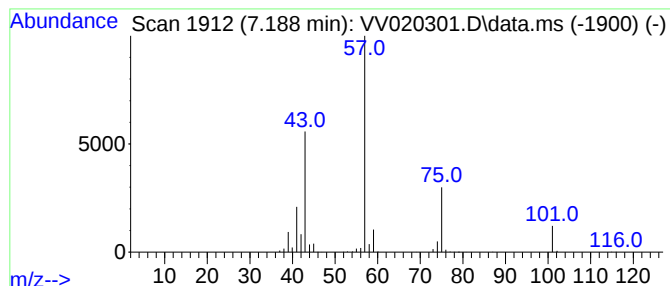
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.188	17.25 ug/L	491651	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53



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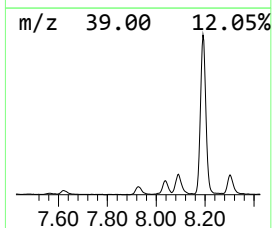
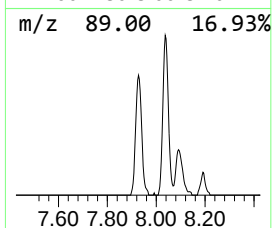
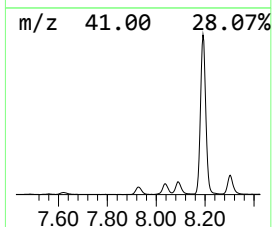
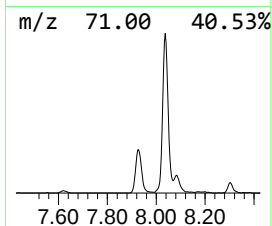
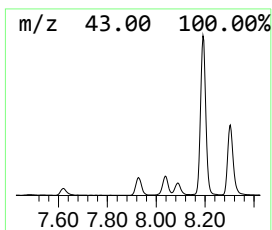
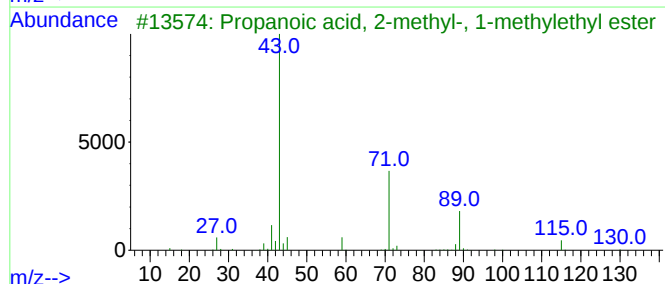
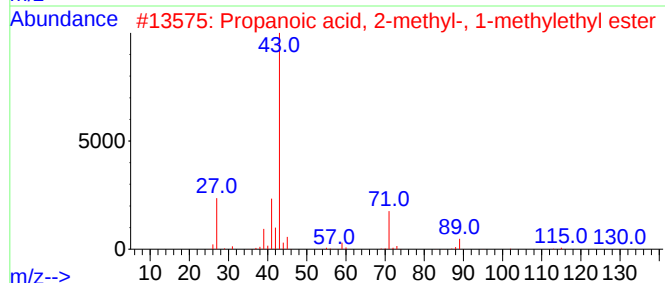
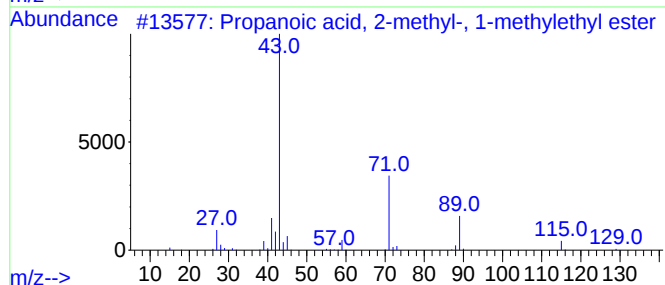
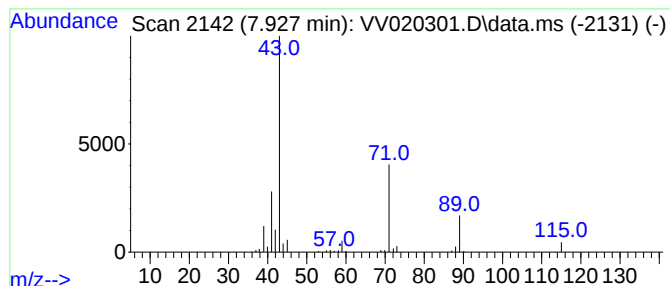
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.927	3.82 ug/L	138416	Chlorobenzene-d5	8.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	64
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
Data File : VV020301.D
Acq On : 11 Feb 2021 16:29
Operator : SY/MD
Sample : PB134573TB
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB01

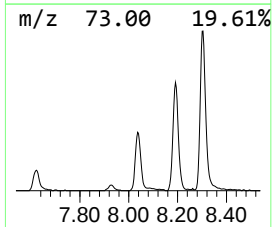
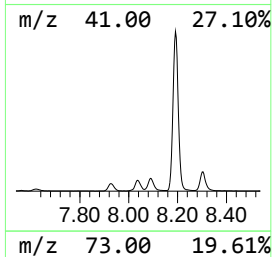
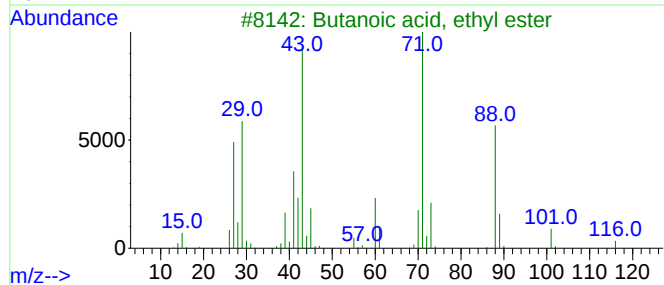
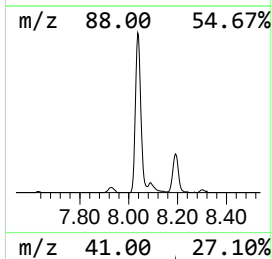
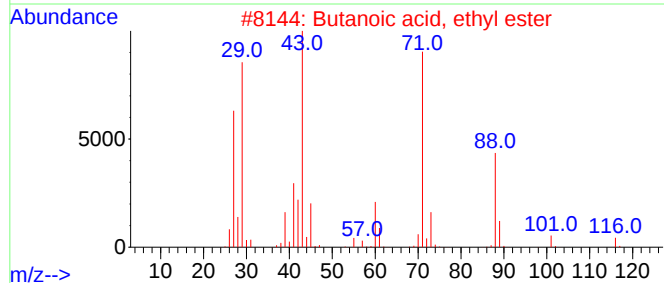
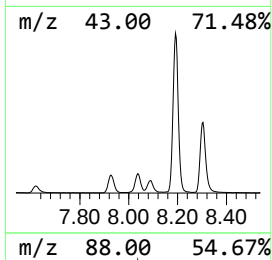
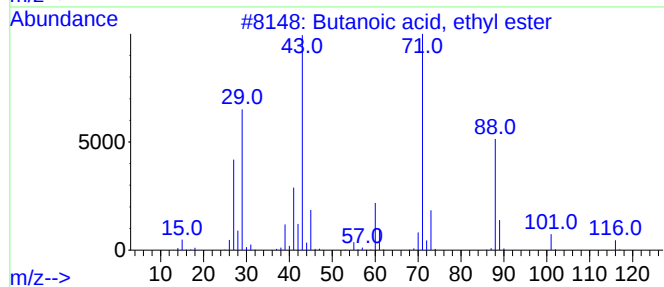
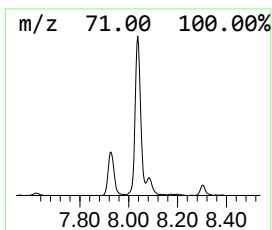
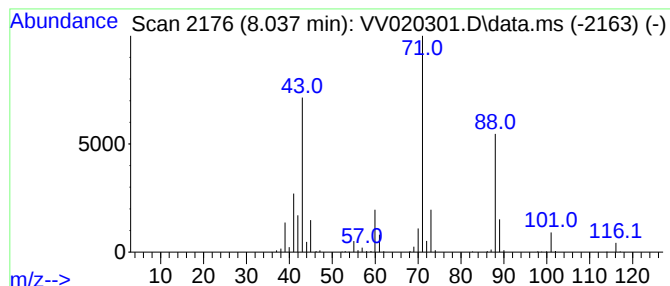
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Quant Title : VOC Analysis

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

Peak Number 5 Butanoic acid, ethyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.037	8.84 ug/L	320526	Chlorobenzene-d5	8.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	91
3			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	64
4			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	47
5			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
Data File : VV020301.D
Acq On : 11 Feb 2021 16:29
Operator : SY/MD
Sample : PB134573TB
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB01

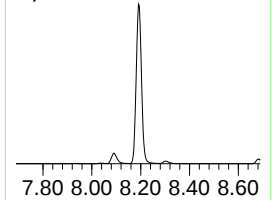
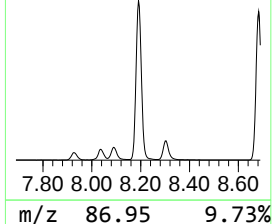
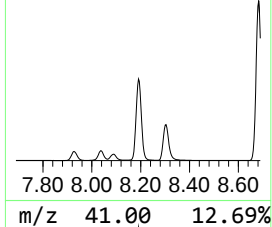
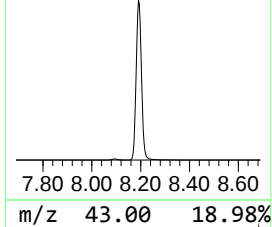
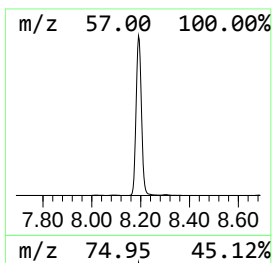
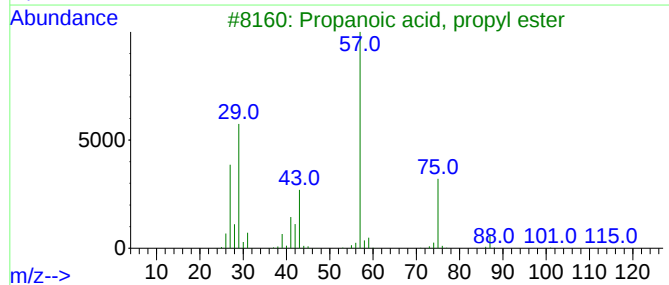
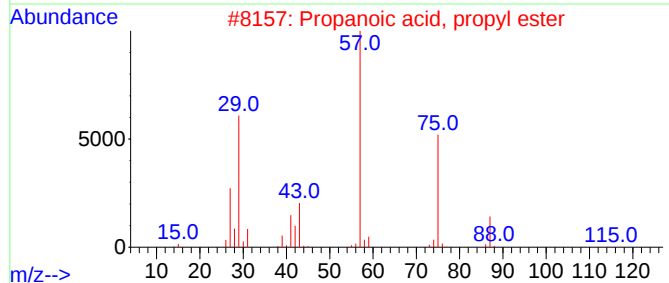
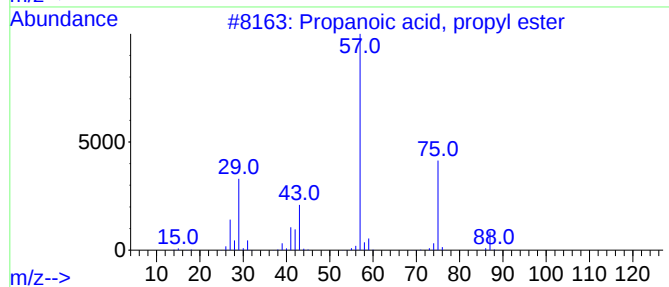
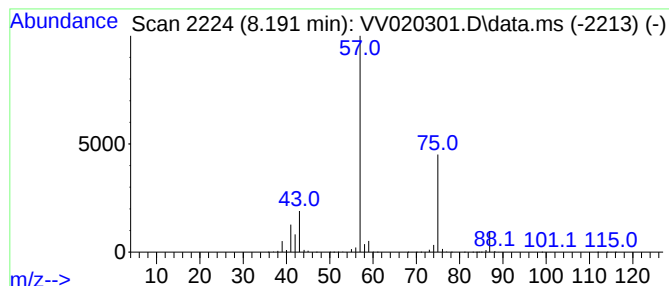
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Quant Title : VOC Analysis

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

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.191	145.04 ug/L	5256920	Chlorobenzene-d5	8.857

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
Data File : VV020301.D
Acq On : 11 Feb 2021 16:29
Operator : SY/MD
Sample : PB134573TB
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB01

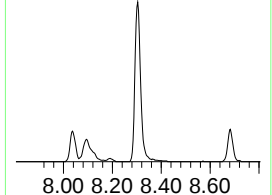
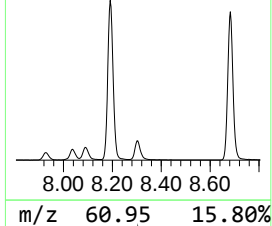
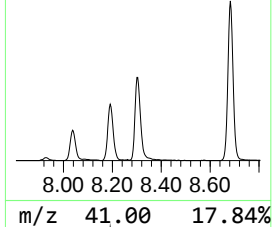
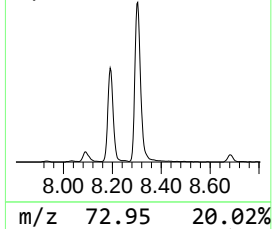
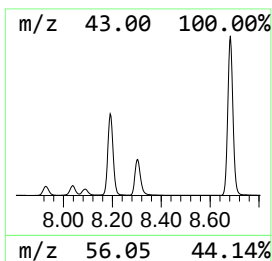
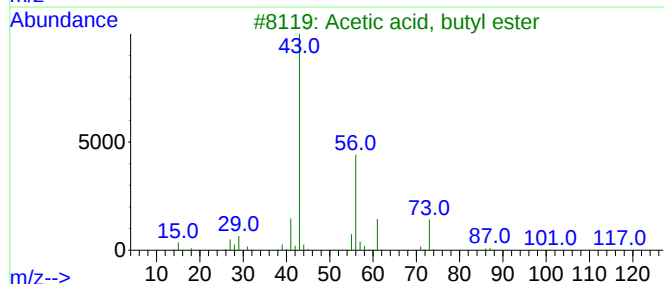
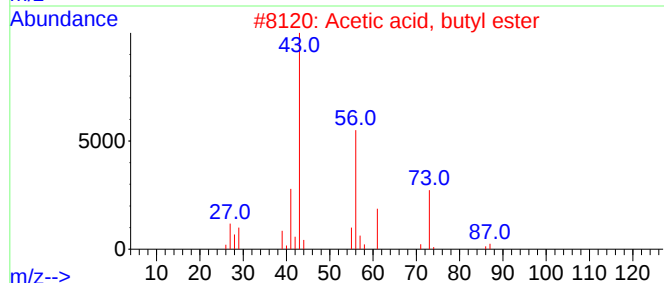
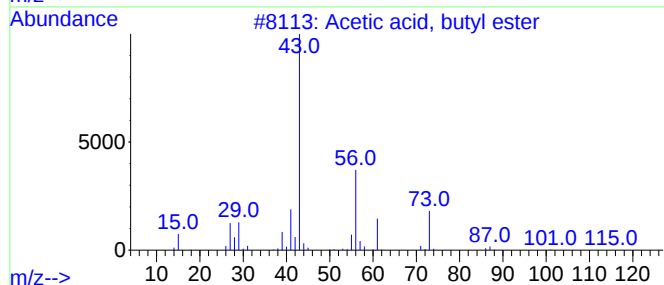
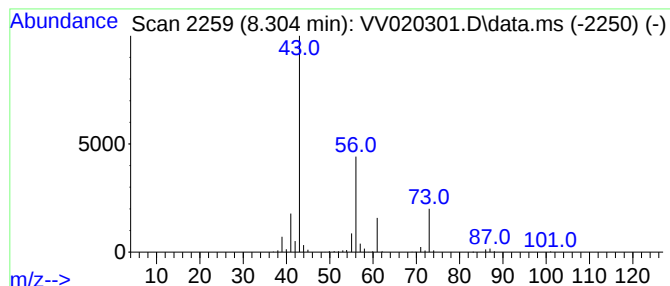
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Quant Title : VOC Analysis

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

Peak Number 7 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.304	14.41 ug/L	522437	Chlorobenzene-d5	8.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	83	
2	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	72	
3	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	72	
4	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	56	
5	Isobutyl acetate		116	C6H12O2	000110-19-0	40	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
Data File : VV020301.D
Acq On : 11 Feb 2021 16:29
Operator : SY/MD
Sample : PB134573TB
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB01

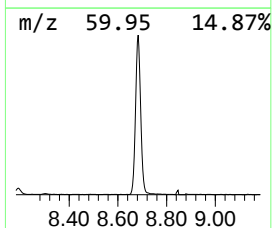
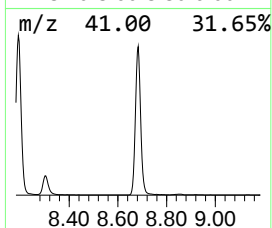
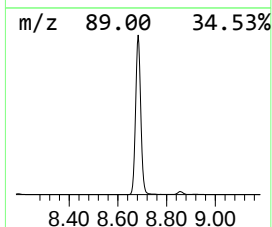
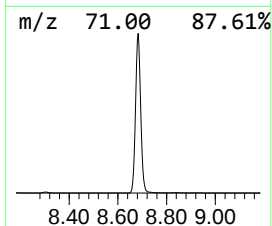
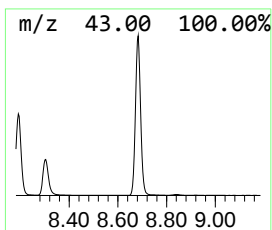
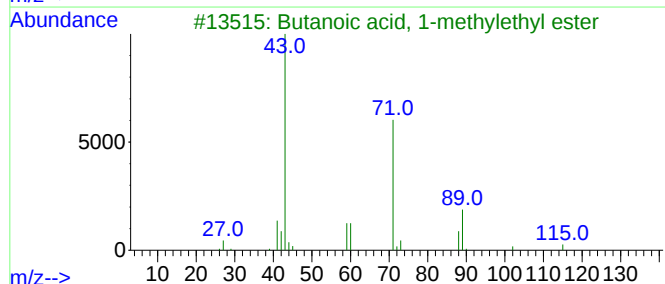
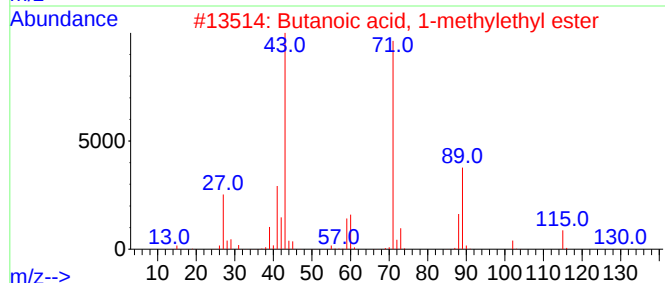
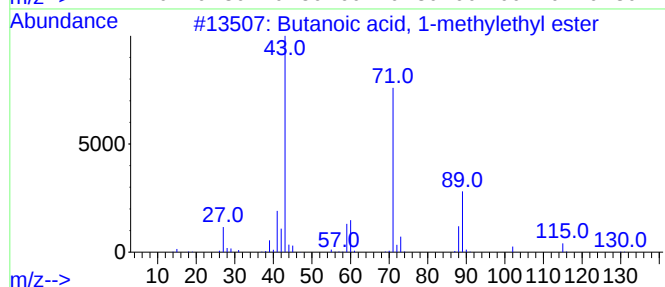
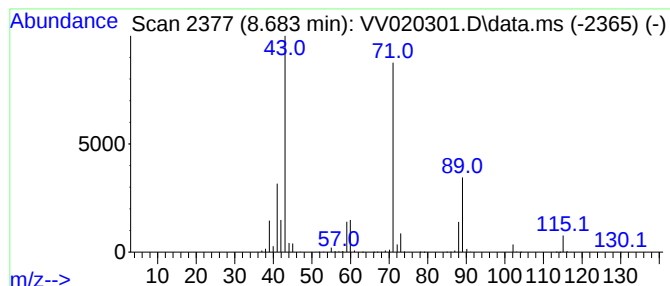
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Quant Title : VOC Analysis

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

Peak Number 8 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.683	88.72 ug/L	3215650	Chlorobenzene-d5	8.857

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	91
3			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	83
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_V\Data\VV021121\
Data File : VV020301.D
Acq On : 11 Feb 2021 16:29
Operator : SY/MD
Sample : PB134573TB
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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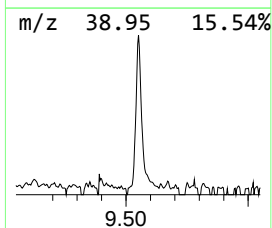
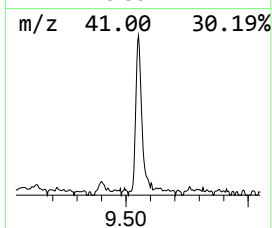
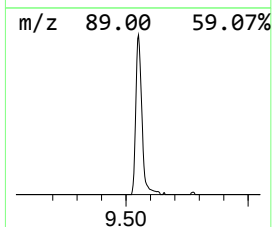
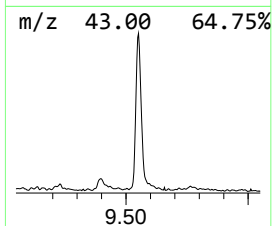
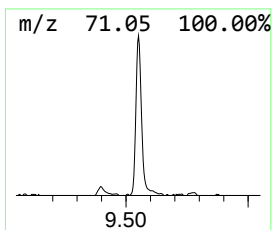
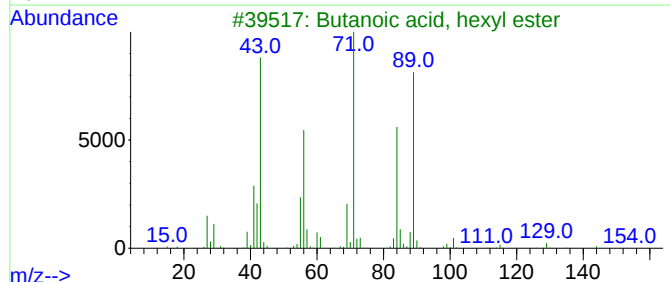
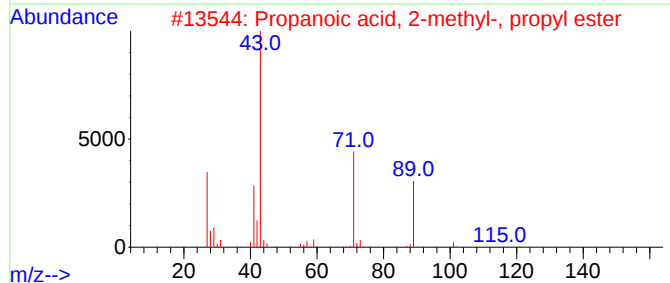
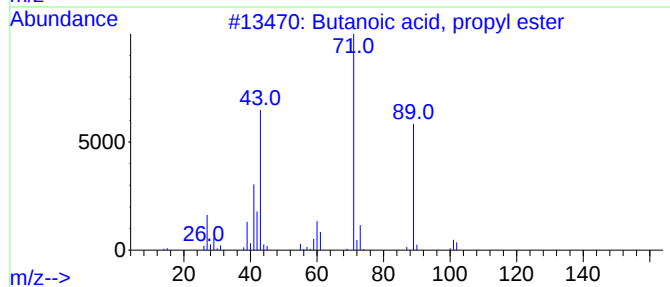
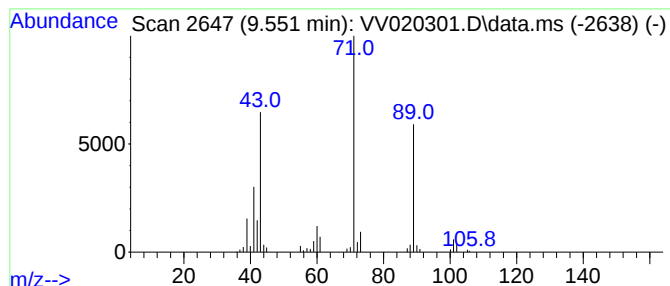
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Quant Title : VOC Analysis

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

Peak Number 9 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.551	2.82 ug/L	102309	Chlorobenzene-d5	8.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2			Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	72
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	72
4			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	72
5			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
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Operator : SY/MD
Sample : PB134573TB
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.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
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Propanoic acid,...	7.188	17.3	ug/L	491651	1	5.619	1425440	50.0
Propanoic acid,...	7.927	3.8	ug/L	138416	2	8.857	1812220	50.0
Butanoic acid, ...	8.037	8.8	ug/L	320526	2	8.857	1812220	50.0
Propanoic acid,...	8.191	145.0	ug/L	5256920	2	8.857	1812220	50.0
Acetic acid, bu...	8.304	14.4	ug/L	522437	2	8.857	1812220	50.0
Butanoic acid, ...	8.683	88.7	ug/L	3215650	2	8.857	1812220	50.0
Butanoic acid, ...	9.551	2.8	ug/L	102309	2	8.857	1812220	50.0