

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
 Data File : VV027063.D
 Acq On : 29 Jul 2022 02:57
 Operator : SY/MD
 Sample : PB146515TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB515

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\SFAMVLM072822WMA.M

Title : VOC Analysis

Signal : TIC: VV027063.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	74	82	101	rVB	334895	359771	15.30%	2.023%
2	1.564	155	163	176	rBV	281401	324569	13.80%	1.825%
3	2.101	319	330	346	rBV	577643	820487	34.89%	4.613%
4	2.500	445	454	466	rBV2	19006	32080	1.36%	0.180%
5	2.613	479	489	490	rBV5	2769	3415	0.15%	0.019%
6	2.677	505	509	512	rBV3	496	415	0.02%	0.002%
7	2.902	577	579	585	rVB3	328	286	0.01%	0.002%
8	3.172	659	663	666	rBV2	394	334	0.01%	0.002%
9	3.256	684	689	693	rBV2	340	303	0.01%	0.002%
10	3.285	695	698	702	rBV2	385	305	0.01%	0.002%
11	3.497	761	764	768	rVV	352	284	0.01%	0.002%
12	3.526	771	773	779	rVV3	363	333	0.01%	0.002%
13	3.783	847	853	856	rBV3	396	409	0.02%	0.002%
14	3.889	868	886	918	rBV3	102971	419081	17.82%	2.356%
15	4.343	1011	1027	1051	rBV	373842	923548	39.27%	5.192%
16	4.638	1115	1119	1125	rVB3	453	462	0.02%	0.003%
17	4.687	1128	1134	1135	rBV2	541	365	0.02%	0.002%
18	4.786	1162	1165	1171	rVB5	492	552	0.02%	0.003%
19	4.854	1184	1186	1193	rVB3	635	511	0.02%	0.003%
20	5.043	1226	1245	1292	rBV2	895350	2351831	100.00%	13.222%
21	5.288	1312	1321	1341	rBV3	10299	26260	1.12%	0.148%
22	5.526	1391	1395	1398	rBV5	477	435	0.02%	0.002%
23	5.545	1398	1401	1405	rVB2	715	430	0.02%	0.002%
24	5.613	1409	1422	1454	rBV	570401	1328885	56.50%	7.471%
25	6.066	1550	1563	1594	rVB	514569	1068558	45.44%	6.007%
26	6.349	1646	1651	1654	rBV3	3986	4749	0.20%	0.027%
27	6.465	1677	1687	1723	rBV	151011	343383	14.60%	1.931%
28	6.982	1837	1848	1881	rBV	233220	448638	19.08%	2.522%
29	7.185	1902	1911	1931	rBV2	34650	68369	2.91%	0.384%
30	7.313	1939	1951	1992	rBV	989743	1775415	75.49%	9.981%
31	7.619	2035	2046	2078	rBV3	200688	384287	16.34%	2.160%
32	7.767	2091	2092	2095	rVB2	1119	309	0.01%	0.002%
33	7.841	2113	2115	2118	rBV4	590	460	0.02%	0.003%
34	7.924	2131	2141	2154	rBV	40791	73705	3.13%	0.414%
35	8.040	2170	2177	2182	rBV5	7469	10583	0.45%	0.059%
36	8.088	2182	2192	2217	rVV	483665	1096884	46.64%	6.167%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
 Title : VOC Analysis

37	8.191	2218	2224	2250	rVV	93297	180844	7.69%	1.017%
38	8.304	2251	2259	2284	rVB2	45342	88803	3.78%	0.499%
39	8.616	2352	2356	2363	rVB7	1111	1330	0.06%	0.007%
40	8.680	2363	2376	2383	rBV	136236	220132	9.36%	1.238%
41	8.850	2417	2429	2457	rBV	931225	1544127	65.66%	8.681%
42	9.114	2508	2511	2513	rBV4	1129	814	0.03%	0.005%
43	9.246	2550	2552	2555	rVB	592	338	0.01%	0.002%
44	9.272	2557	2560	2562	rVB3	625	282	0.01%	0.002%
45	9.284	2562	2564	2565	rBV2	796	288	0.01%	0.002%
46	9.336	2577	2580	2582	rBV2	541	292	0.01%	0.002%
47	9.384	2592	2595	2596	rBV2	798	517	0.02%	0.003%
48	9.551	2638	2647	2657	rBV3	9217	15749	0.67%	0.089%
49	9.632	2671	2672	2675	rVB2	988	359	0.02%	0.002%
50	9.760	2707	2712	2715	rBV4	608	586	0.02%	0.003%
51	9.844	2736	2738	2742	rVB2	435	280	0.01%	0.002%
52	9.870	2742	2746	2747	rBV2	406	277	0.01%	0.002%
53	9.915	2756	2760	2762	rBV2	540	424	0.02%	0.002%
54	9.931	2762	2765	2767	rBV	564	350	0.01%	0.002%
55	9.966	2772	2776	2782	rBV2	448	591	0.03%	0.003%
56	9.995	2782	2785	2786	rBV2	451	308	0.01%	0.002%
57	10.214	2840	2853	2873	rBV	746901	1200010	51.02%	6.746%
58	10.349	2891	2895	2902	rVB2	671	796	0.03%	0.004%
59	10.432	2919	2921	2924	rVB	596	303	0.01%	0.002%
60	10.545	2952	2956	2962	rVB3	667	579	0.02%	0.003%
61	10.574	2962	2965	2968	rBV2	780	525	0.02%	0.003%
62	10.635	2980	2984	2986	rBV2	436	317	0.01%	0.002%
63	10.648	2986	2988	2994	rVB2	444	339	0.01%	0.002%
64	10.690	2994	3001	3003	rBV4	524	581	0.02%	0.003%
65	10.754	3017	3021	3024	rBV2	636	520	0.02%	0.003%
66	10.956	3082	3084	3087	rBV	403	278	0.01%	0.002%
67	10.976	3087	3090	3092	rVB2	450	276	0.01%	0.002%
68	11.085	3121	3124	3128	rVB3	466	383	0.02%	0.002%
69	11.169	3146	3150	3153	rBV4	398	417	0.02%	0.002%
70	11.249	3160	3175	3197	rBV	793624	1232144	52.39%	6.927%
71	11.622	3279	3291	3312	rBV	891192	1410190	59.96%	7.928%
72	11.905	3376	3379	3384	rVB4	521	550	0.02%	0.003%
73	12.075	3429	3432	3436	rVB3	371	338	0.01%	0.002%
74	12.252	3484	3487	3490	rVB2	630	447	0.02%	0.003%
75	12.316	3505	3507	3510	rVB3	601	312	0.01%	0.002%
76	12.448	3545	3548	3552	rBV2	336	331	0.01%	0.002%

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Integrator: RTE

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
 Title : VOC Analysis

77	12.558	3580	3582	3585	rBV2	414	270	0.01%	0.002%
78	12.651	3608	3611	3614	rBV4	450	311	0.01%	0.002%
79	12.709	3625	3629	3632	rBV	445	332	0.01%	0.002%
80	12.741	3636	3639	3644	rVB3	502	385	0.02%	0.002%
81	12.982	3709	3714	3716	rBV2	370	407	0.02%	0.002%
82	13.226	3786	3790	3795	rBV3	401	430	0.02%	0.002%
83	13.275	3802	3805	3809	rVB4	596	451	0.02%	0.003%
84	13.316	3814	3818	3826	rVB4	605	730	0.03%	0.004%
85	13.394	3840	3842	3849	rVB3	552	477	0.02%	0.003%
86	13.429	3849	3853	3856	rVB2	649	476	0.02%	0.003%
87	13.686	3931	3933	3936	rVB2	614	281	0.01%	0.002%
88	13.760	3954	3956	3961	rVB3	528	400	0.02%	0.002%
89	13.796	3961	3967	3970	rBV2	365	359	0.02%	0.002%
90	13.860	3985	3987	3993	rVB3	520	428	0.02%	0.002%
91	13.966	4016	4020	4022	rBV2	637	534	0.02%	0.003%
92	13.995	4025	4029	4030	rBV	442	282	0.01%	0.002%
93	14.394	4150	4153	4155	rVB3	515	288	0.01%	0.002%
94	14.599	4215	4217	4226	rVV6	450	606	0.03%	0.003%
95	14.770	4266	4270	4273	rBV3	552	430	0.02%	0.002%
96	14.837	4286	4291	4292	rBV4	679	522	0.02%	0.003%
97	14.931	4317	4320	4324	rBV4	734	738	0.03%	0.004%
98	15.162	4389	4392	4397	rBV3	490	418	0.02%	0.002%
99	15.223	4408	4411	4413	rBV3	592	340	0.01%	0.002%
100	15.358	4451	4453	4459	rVB4	545	340	0.01%	0.002%

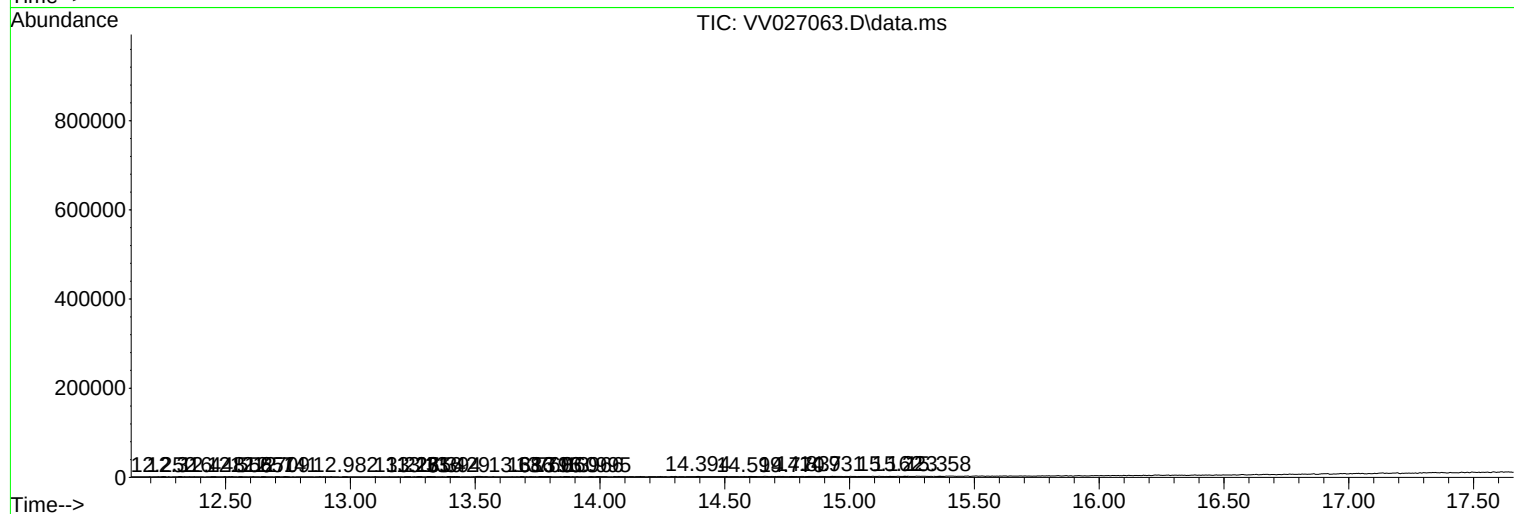
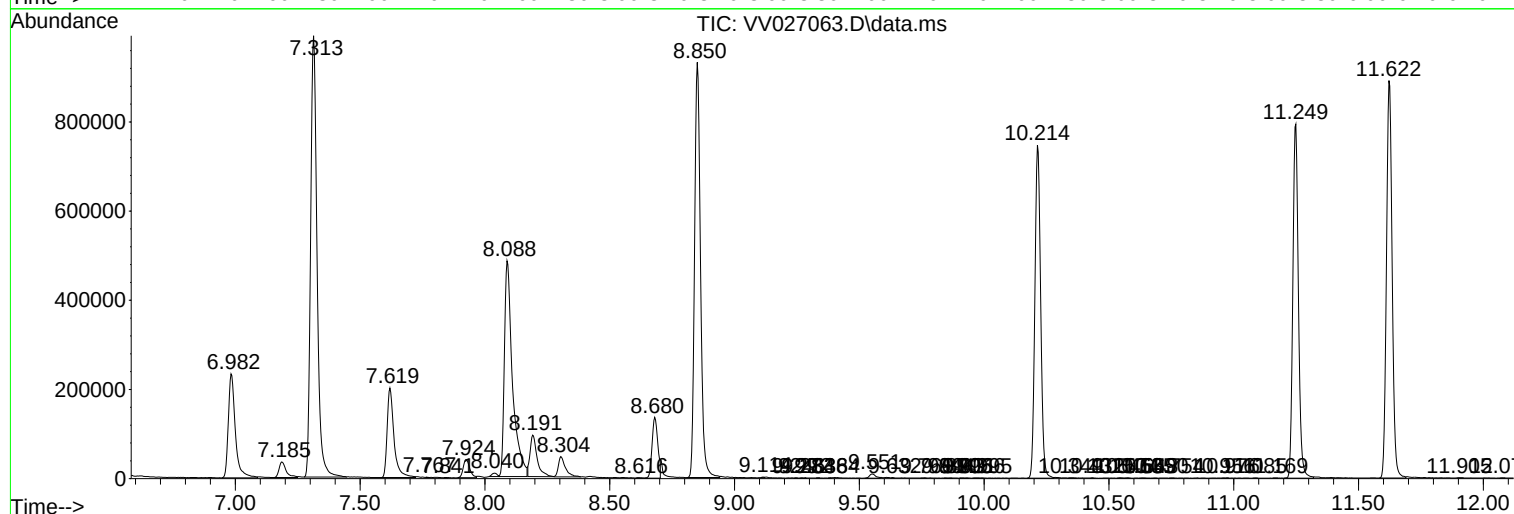
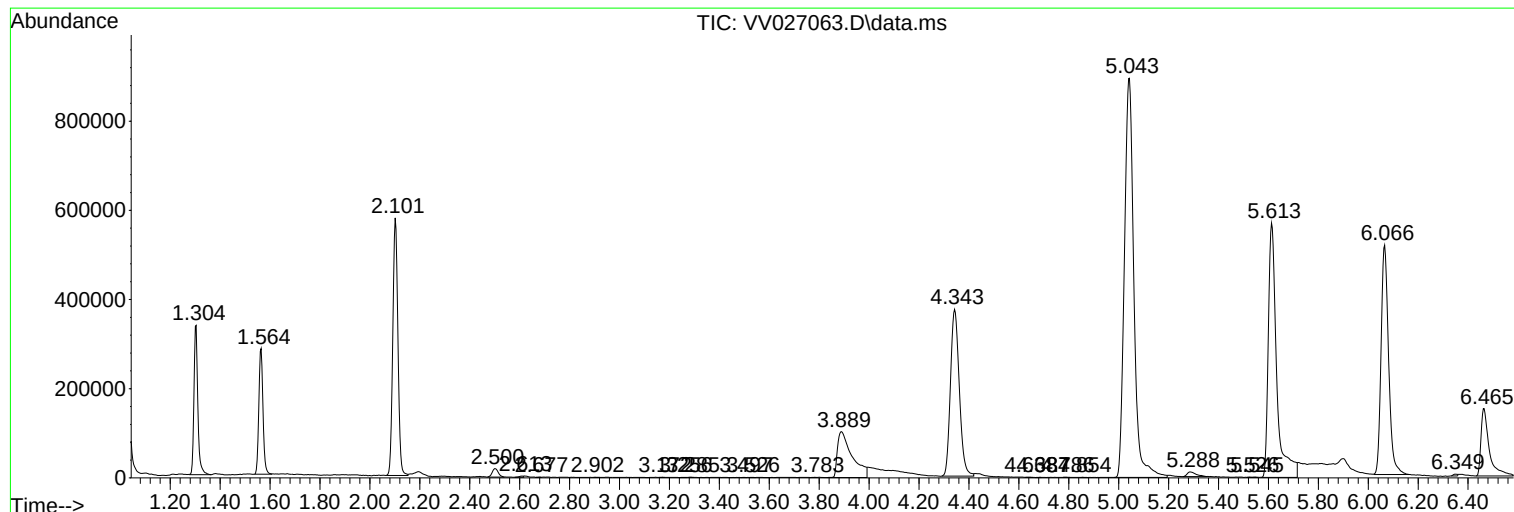
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MSVOA_V
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_V
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VLEB515

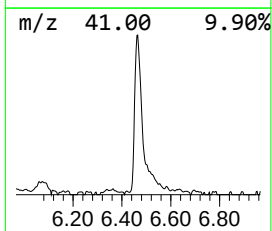
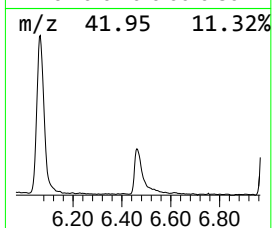
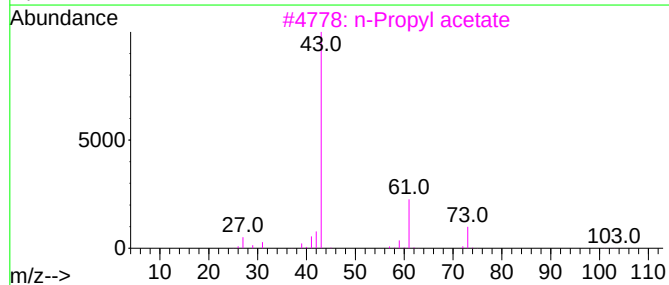
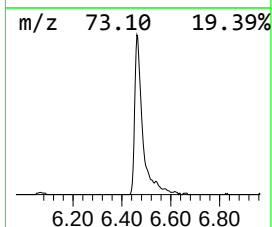
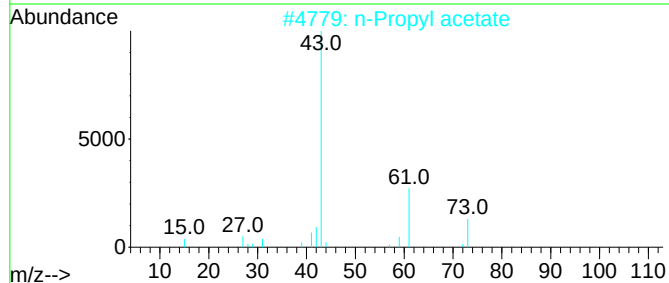
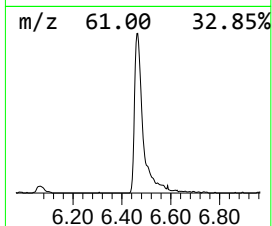
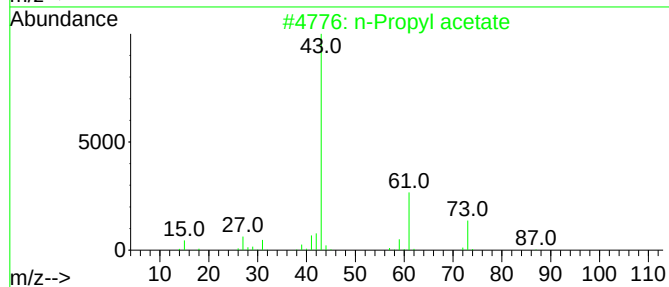
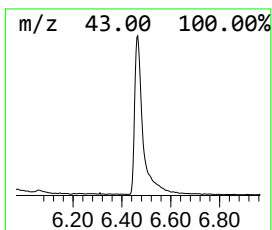
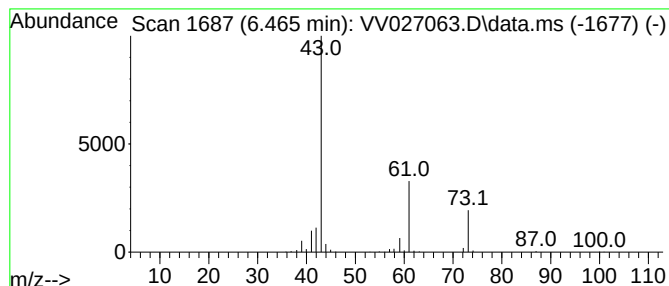
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.465	12.92 ug/L	343383	1,4-Difluorobenzene	5.613

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	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	72



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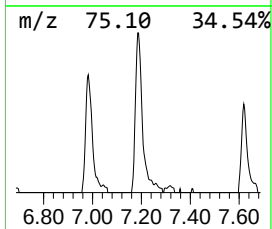
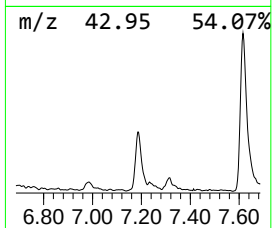
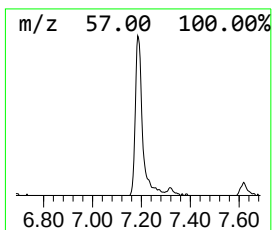
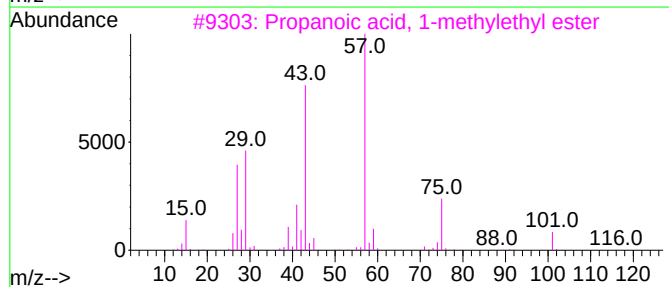
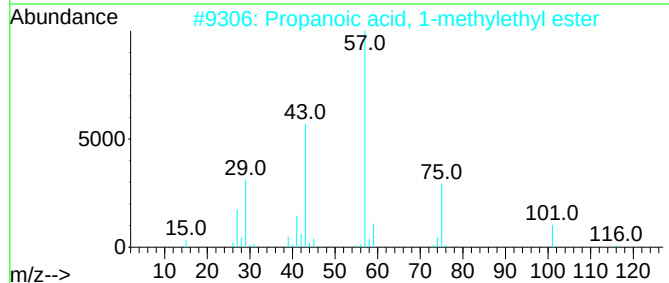
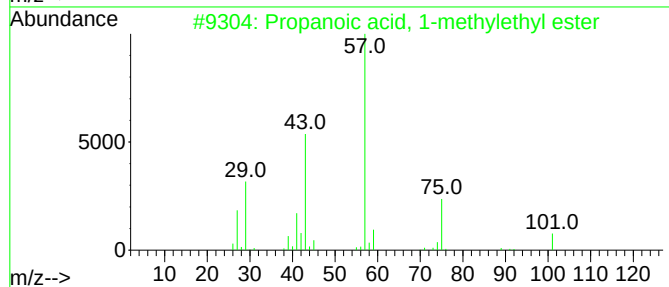
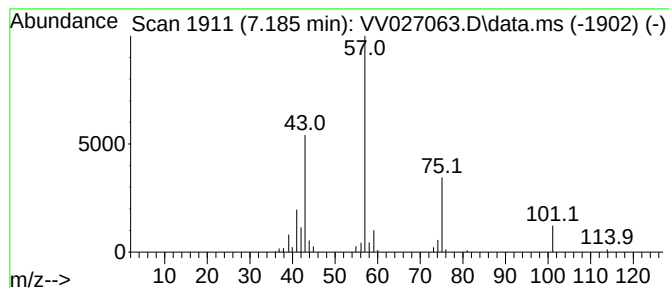
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.185	2.57 ug/L	68369	1,4-Difluorobenzene	5.613

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	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59



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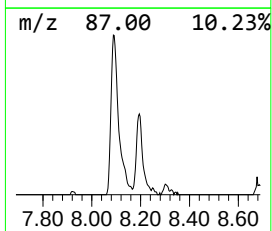
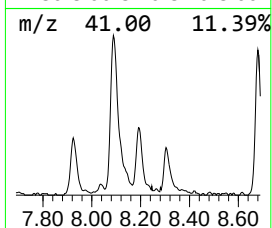
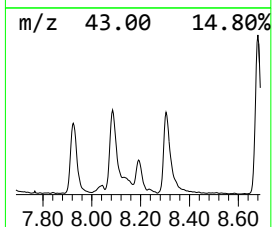
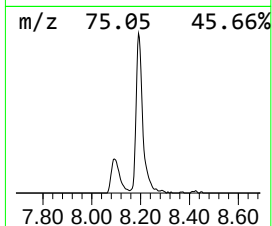
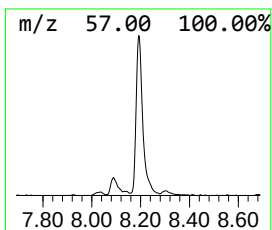
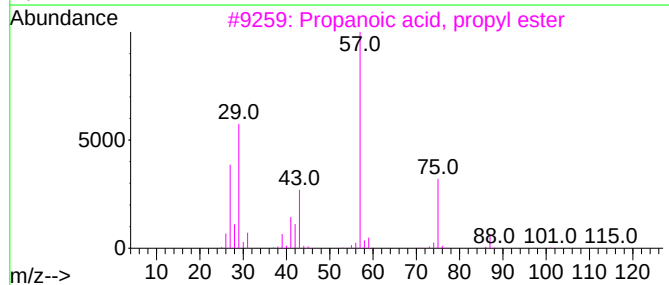
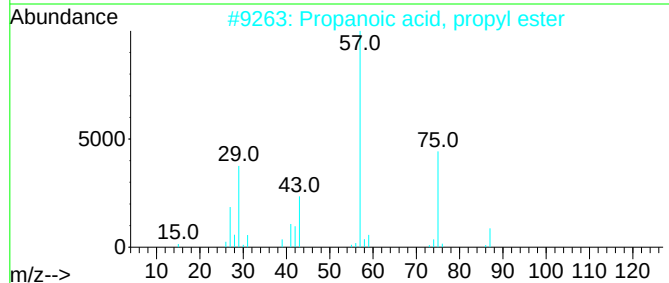
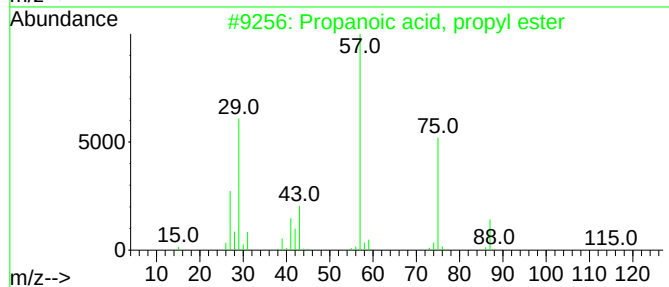
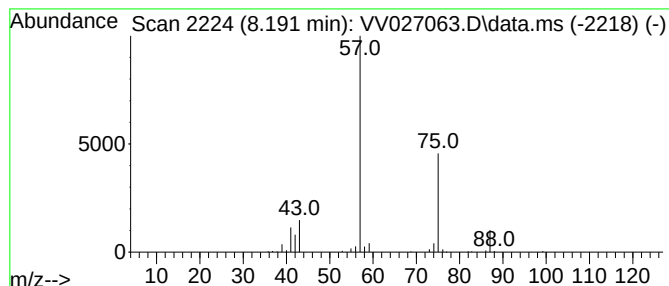
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.191	5.86 ug/L	180844	Chlorobenzene-d5	8.850

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	64
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
Data File : VV027063.D
Acq On : 29 Jul 2022 02:57
Operator : SY/MD
Sample : PB146515TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB515

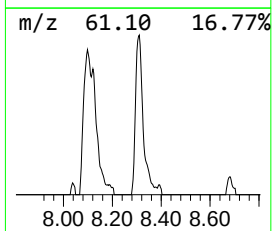
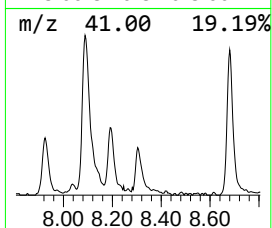
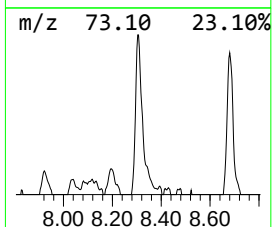
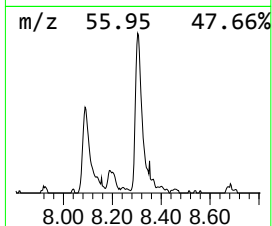
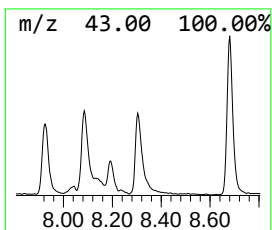
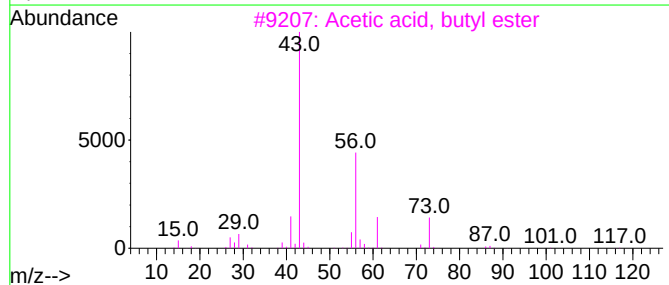
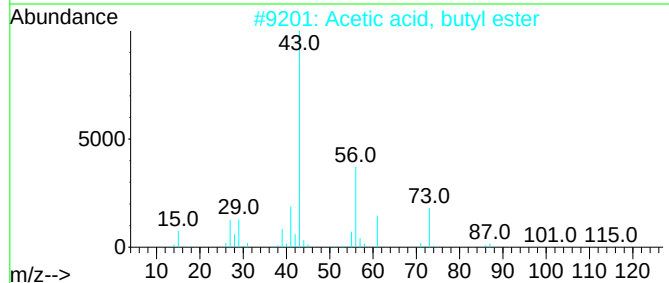
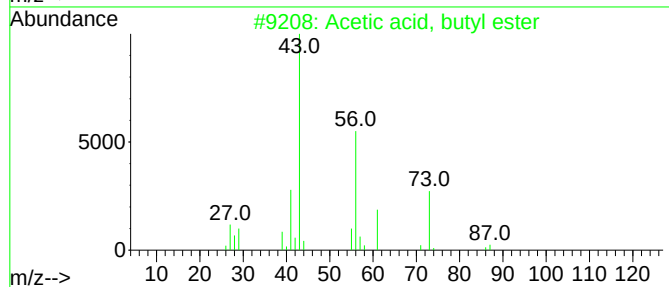
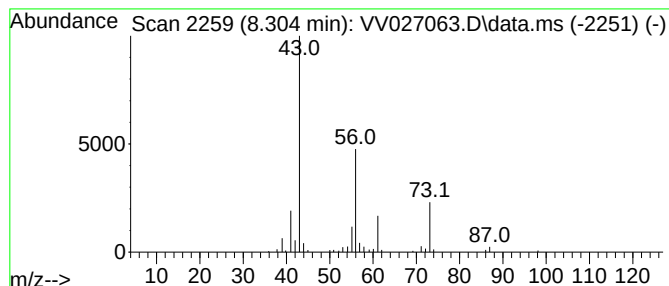
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.304	2.88 ug/L	88803	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	86
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
5			Isobutyl acetate	116	C6H12O2	000110-19-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
Data File : VV027063.D
Acq On : 29 Jul 2022 02:57
Operator : SY/MD
Sample : PB146515TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB515

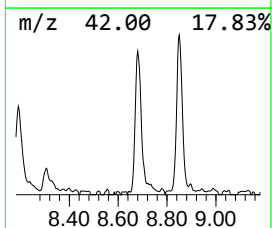
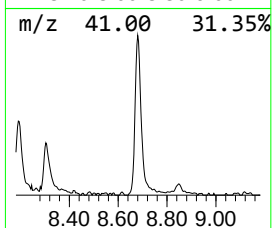
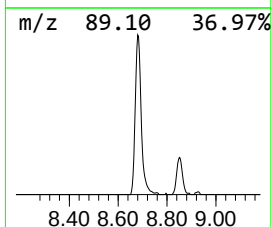
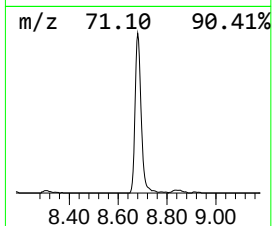
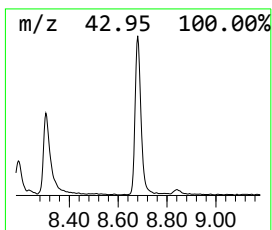
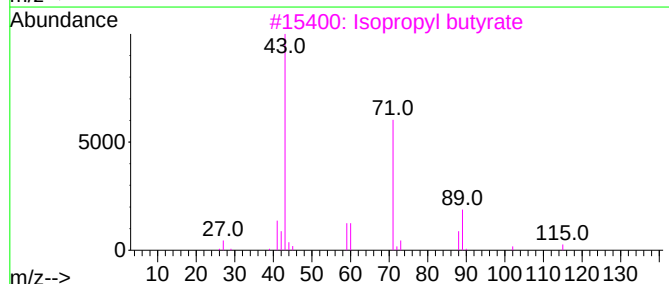
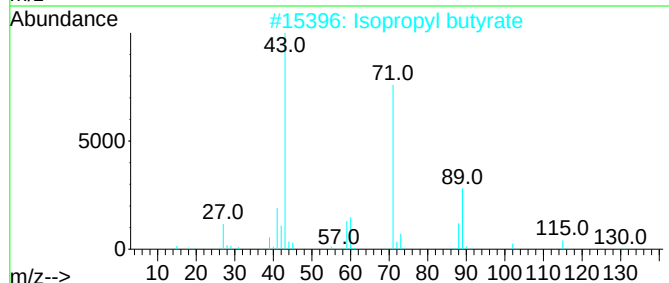
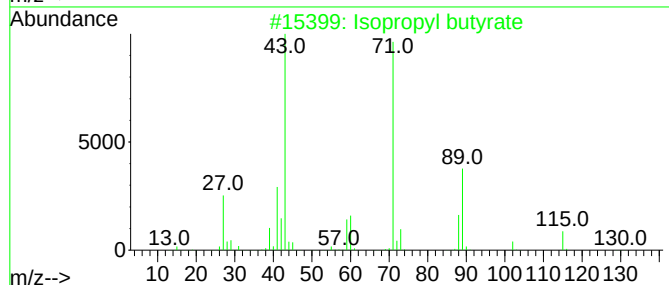
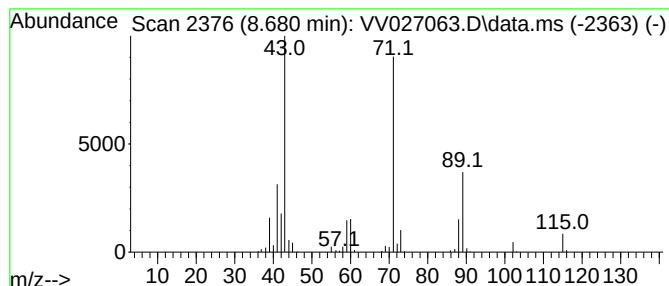
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.680	7.13 ug/L	220132	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78
5			Isopropyl butyrate	130	C7H14O2	000638-11-9	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
Data File : VV027063.D
Acq On : 29 Jul 2022 02:57
Operator : SY/MD
Sample : PB146515TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB515

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.465	12.9	ug/L	343383	1	5.613	1328890	50.0
Propanoic acid,...	7.185	2.6	ug/L	68369	1	5.613	1328890	50.0
Propanoic acid,...	8.191	5.9	ug/L	180844	2	8.850	1544130	50.0
Acetic acid, bu...	8.304	2.9	ug/L	88803	2	8.850	1544130	50.0
Isopropyl butyrate	8.680	7.1	ug/L	220132	2	8.850	1544130	50.0