

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122022\
 Data File : VV029748.D
 Acq On : 20 Dec 2022 14:00
 Operator : SY/MD
 Sample : PB149759TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB759

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\SFAMVLM120722WMA.M
 Title : VOC Analysis

Signal : TIC: VV029748.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	100	rVB	194057	196526	13.82%	1.517%
2	1.565	156	163	177	rVB	172341	194680	13.69%	1.502%
3	1.770	225	227	231	rBV2	797	538	0.04%	0.004%
4	2.105	320	331	343	rBV	328887	471962	33.19%	3.642%
5	2.288	385	388	391	rBV3	719	411	0.03%	0.003%
6	2.503	444	455	468	rVV2	8463	14209	1.00%	0.110%
7	2.587	477	481	487	rBV3	286	357	0.03%	0.003%
8	2.622	487	492	495	rVB2	227	241	0.02%	0.002%
9	2.690	508	513	517	rBV2	330	297	0.02%	0.002%
10	2.886	570	574	576	rBV	285	242	0.02%	0.002%
11	2.966	596	599	605	rVV2	342	249	0.02%	0.002%
12	3.005	605	611	617	rVV3	302	377	0.03%	0.003%
13	3.172	656	663	664	rBV2	1056	895	0.06%	0.007%
14	3.876	871	882	928	rBV	89158	279862	19.68%	2.160%
15	4.339	1008	1026	1052	rBV	221143	556847	39.16%	4.298%
16	4.690	1132	1135	1144	rVB3	324	446	0.03%	0.003%
17	4.741	1144	1151	1152	rBV2	368	367	0.03%	0.003%
18	4.905	1195	1202	1207	rVB2	216	292	0.02%	0.002%
19	5.040	1224	1244	1295	rBV2	531793	1422035	100.00%	10.975%
20	5.281	1304	1319	1336	rBV2	13351	33022	2.32%	0.255%
21	5.378	1346	1349	1352	rBV2	557	327	0.02%	0.003%
22	5.471	1373	1378	1381	rBV3	373	417	0.03%	0.003%
23	5.609	1408	1421	1447	rBV	535693	1086574	76.41%	8.386%
24	5.822	1484	1487	1492	rVB3	618	556	0.04%	0.004%
25	5.902	1501	1512	1523	rBV4	4042	7446	0.52%	0.057%
26	6.063	1547	1562	1592	rBV	310465	650879	45.77%	5.023%
27	6.243	1615	1618	1625	rVB5	534	529	0.04%	0.004%
28	6.349	1642	1651	1674	rBV2	5276	16608	1.17%	0.128%
29	6.461	1676	1686	1715	rBV	157344	314263	22.10%	2.425%
30	6.818	1794	1797	1802	rVB2	370	251	0.02%	0.002%
31	6.918	1825	1828	1832	rBV2	375	366	0.03%	0.003%
32	6.979	1833	1847	1874	rBV	164244	306091	21.52%	2.362%
33	7.182	1897	1910	1934	rBV2	37750	74469	5.24%	0.575%
34	7.307	1937	1949	1977	rBV	644965	1150034	80.87%	8.876%
35	7.613	2033	2044	2073	rBV2	156490	286031	20.11%	2.207%
36	7.767	2090	2092	2097	rVB3	489	343	0.02%	0.003%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
 Title : VOC Analysis

37	7.822	2105	2109	2114	rVB4	662	470	0.03%	0.004%
38	7.863	2118	2122	2126	rBV3	372	294	0.02%	0.002%
39	7.918	2126	2139	2158	rBV	51908	91521	6.44%	0.706%
40	8.031	2160	2174	2180	rVV6	9065	17985	1.26%	0.139%
41	8.085	2180	2191	2214	rVV	352324	674387	47.42%	5.205%
42	8.188	2215	2223	2247	rVV	91761	164535	11.57%	1.270%
43	8.297	2248	2257	2280	rVB	51985	92084	6.48%	0.711%
44	8.471	2306	2311	2313	rBV5	552	542	0.04%	0.004%
45	8.674	2361	2374	2396	rBV	158633	262070	18.43%	2.023%
46	8.844	2414	2427	2452	rBV	805652	1327800	93.37%	10.248%
47	9.021	2480	2482	2485	rVB2	687	415	0.03%	0.003%
48	9.059	2492	2494	2498	rVB3	514	252	0.02%	0.002%
49	9.111	2503	2510	2524	rVB5	1819	3693	0.26%	0.029%
50	9.256	2551	2555	2561	rVB4	561	488	0.03%	0.004%
51	9.378	2585	2593	2594	rBV3	1796	1375	0.10%	0.011%
52	9.420	2603	2606	2609	rVB2	683	430	0.03%	0.003%
53	9.542	2635	2644	2659	rVV	14715	22361	1.57%	0.173%
54	9.747	2706	2708	2714	rVB2	463	298	0.02%	0.002%
55	9.857	2737	2742	2747	rBV2	355	384	0.03%	0.003%
56	9.902	2751	2756	2758	rBV	379	244	0.02%	0.002%
57	9.966	2772	2776	2779	rBV2	344	293	0.02%	0.002%
58	10.098	2814	2817	2826	rVB3	519	567	0.04%	0.004%
59	10.162	2826	2837	2840	rBV2	7239	9939	0.70%	0.077%
60	10.204	2840	2850	2878	rVB	457879	730065	51.34%	5.634%
61	10.368	2894	2901	2909	rBV6	2294	3715	0.26%	0.029%
62	10.461	2927	2930	2934	rVB2	283	244	0.02%	0.002%
63	10.493	2936	2940	2945	rBV2	195	254	0.02%	0.002%
64	10.526	2948	2950	2953	rBV2	465	342	0.02%	0.003%
65	10.571	2957	2964	2974	rVV3	3586	5341	0.38%	0.041%
66	10.780	3024	3029	3031	rBV2	249	231	0.02%	0.002%
67	10.998	3090	3097	3101	rBV2	372	422	0.03%	0.003%
68	11.140	3136	3141	3143	rBV3	323	284	0.02%	0.002%
69	11.236	3158	3171	3195	rBV	840924	1323242	93.05%	10.212%
70	11.468	3240	3243	3246	rVB2	505	346	0.02%	0.003%
71	11.516	3255	3258	3259	rBV2	431	288	0.02%	0.002%
72	11.548	3261	3268	3276	rVV7	3678	6827	0.48%	0.053%
73	11.612	3276	3288	3310	rVV	705385	1087142	76.45%	8.390%
74	11.770	3334	3337	3341	rBV4	396	345	0.02%	0.003%
75	11.847	3358	3361	3366	rVB3	474	362	0.03%	0.003%
76	11.905	3377	3379	3382	rVB	624	267	0.02%	0.002%

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77	11.940	3387	3390	3395	rVB3	428	373	0.03%	0.003%
78	11.989	3401	3405	3408	rBV3	462	338	0.02%	0.003%
79	12.117	3441	3445	3447	rBV2	511	419	0.03%	0.003%
80	12.175	3461	3463	3469	rVB2	346	280	0.02%	0.002%
81	12.210	3469	3474	3477	rBV	622	612	0.04%	0.005%
82	12.239	3477	3483	3492	rVB4	1619	2358	0.17%	0.018%
83	12.410	3534	3536	3540	rVB2	549	311	0.02%	0.002%
84	12.587	3587	3591	3595	rBV3	422	384	0.03%	0.003%
85	12.628	3603	3604	3609	rVB3	533	292	0.02%	0.002%
86	12.831	3658	3667	3680	rBV9	4535	8276	0.58%	0.064%
87	12.947	3698	3703	3710	rVB3	2355	2630	0.18%	0.020%
88	13.082	3740	3745	3751	rVB2	2580	2535	0.18%	0.020%
89	13.185	3774	3777	3783	rVB5	386	407	0.03%	0.003%
90	13.345	3824	3827	3832	rBV3	516	476	0.03%	0.004%
91	13.493	3871	3873	3875	rBV3	544	289	0.02%	0.002%
92	13.580	3897	3900	3902	rBV2	551	366	0.03%	0.003%
93	13.731	3944	3947	3953	rVB4	780	747	0.05%	0.006%
94	13.760	3954	3956	3959	rBV3	458	314	0.02%	0.002%
95	13.818	3969	3974	3980	rBV4	606	790	0.06%	0.006%
96	13.943	4010	4013	4014	rBV2	422	276	0.02%	0.002%
97	14.394	4150	4153	4156	rBV2	801	627	0.04%	0.005%
98	14.802	4273	4280	4287	rBV8	4002	5657	0.40%	0.044%
99	14.886	4302	4306	4307	rBV3	1904	1323	0.09%	0.010%
100	15.760	4571	4578	4587	rVB3	18811	26008	1.83%	0.201%

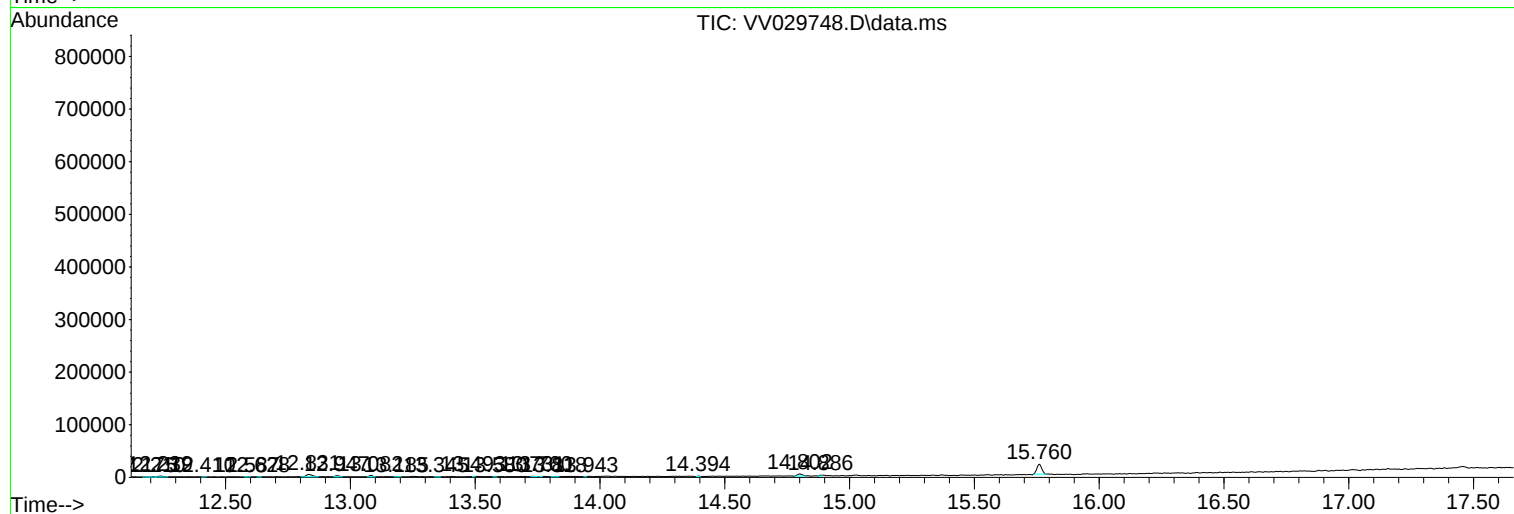
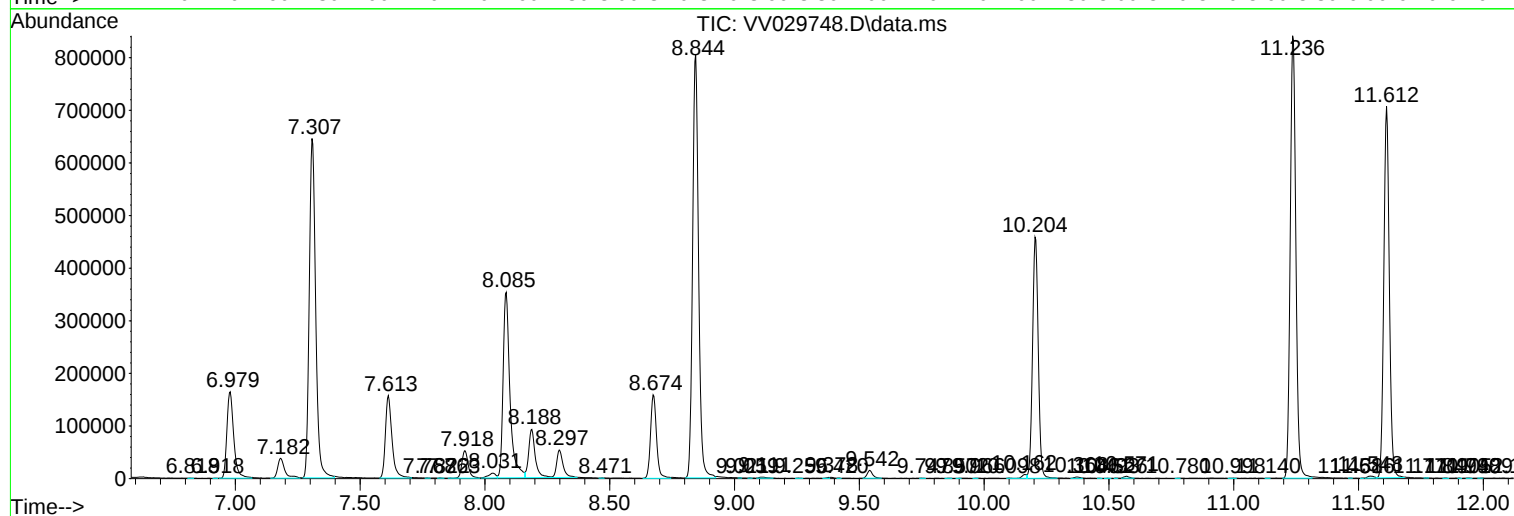
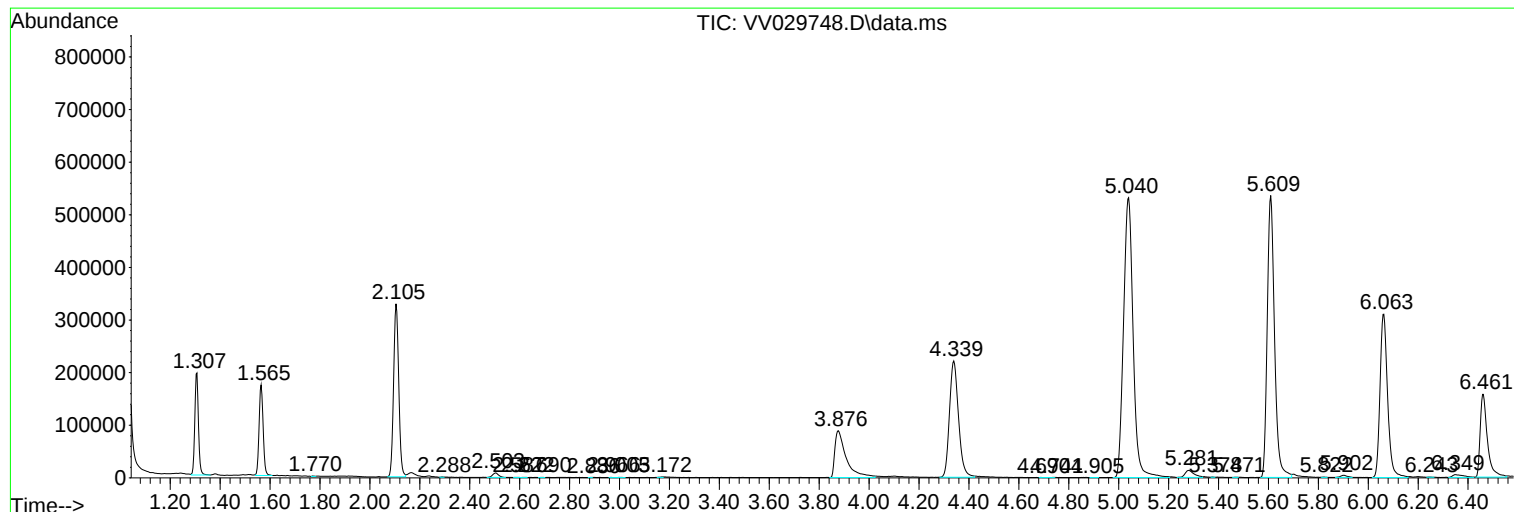
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB759

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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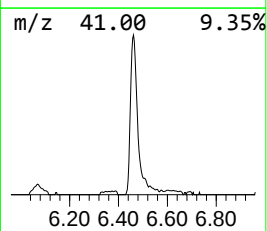
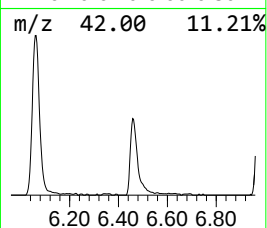
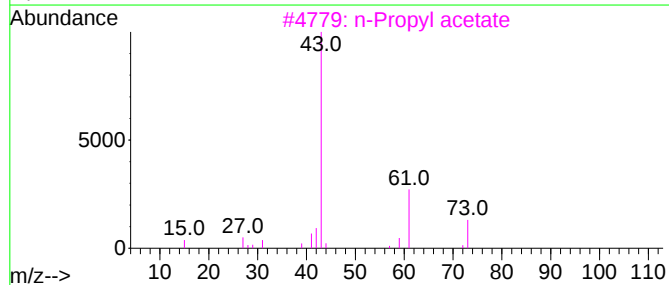
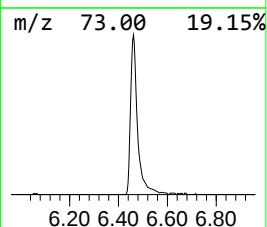
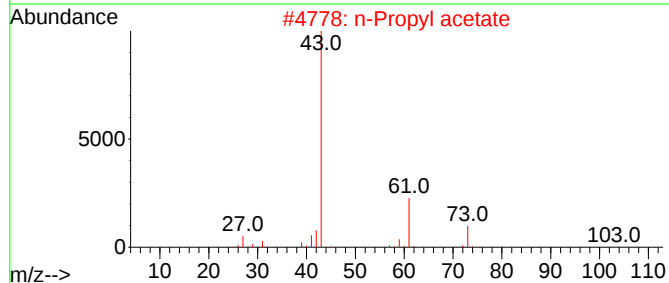
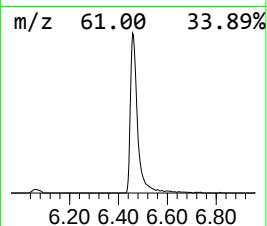
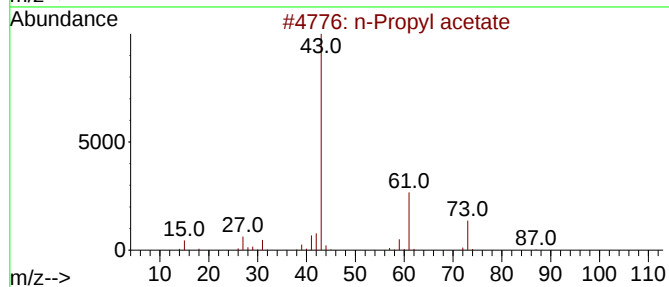
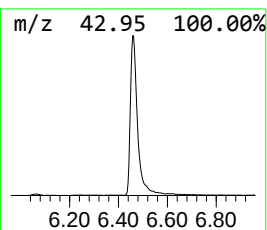
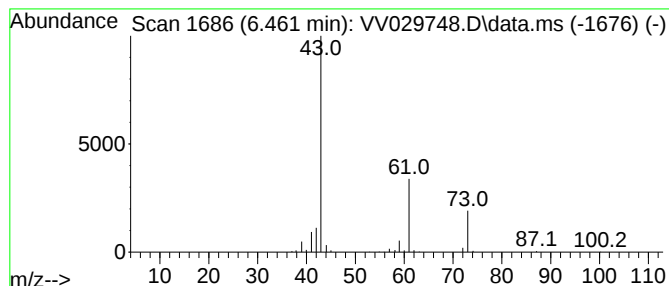
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.461	14.46 ug/L	314263	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	83
3		n-Propyl acetate	102	C5H10O2	000109-60-4	78
4		n-Propyl acetate	102	C5H10O2	000109-60-4	72
5		Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	38



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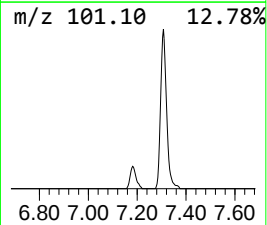
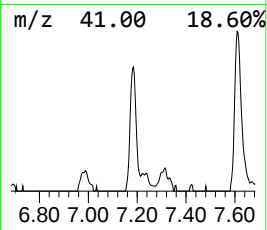
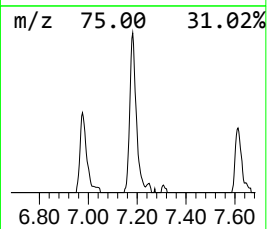
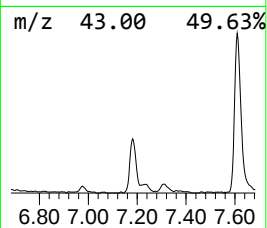
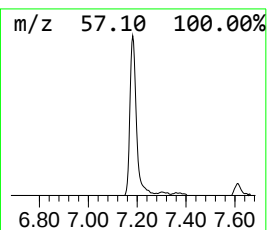
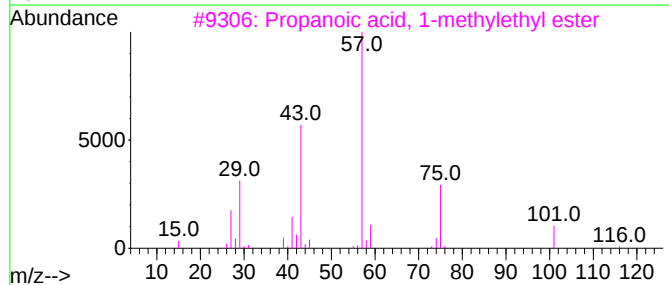
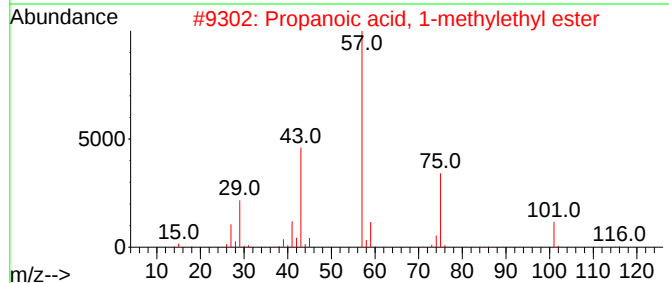
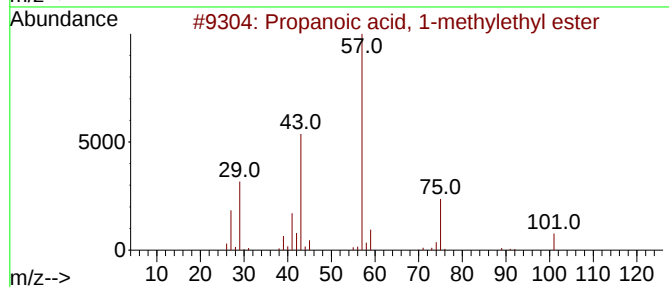
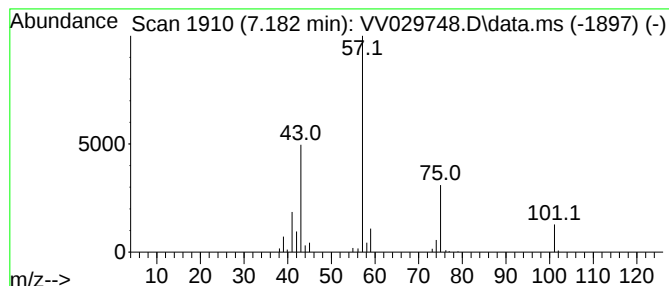
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Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.182	3.43 ug/L	74469	1,4-Difluorobenzene	5.609

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	83
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59



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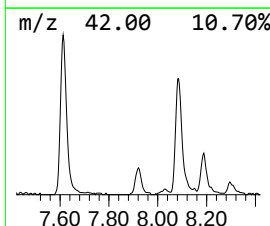
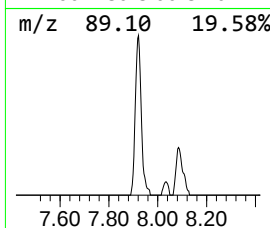
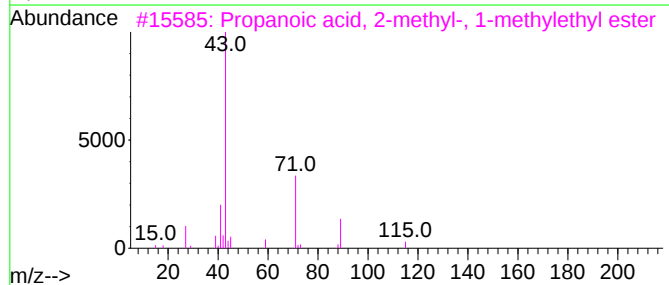
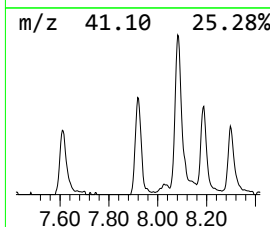
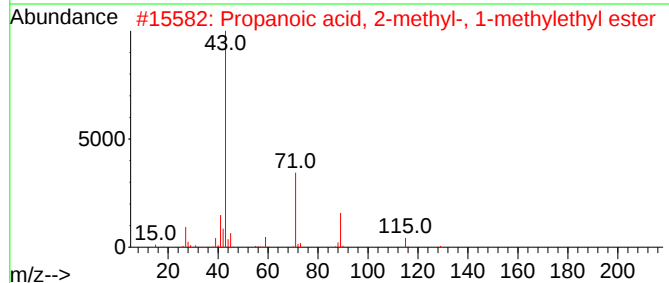
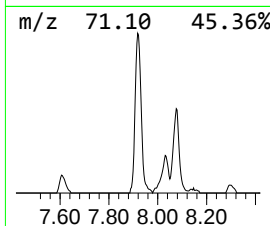
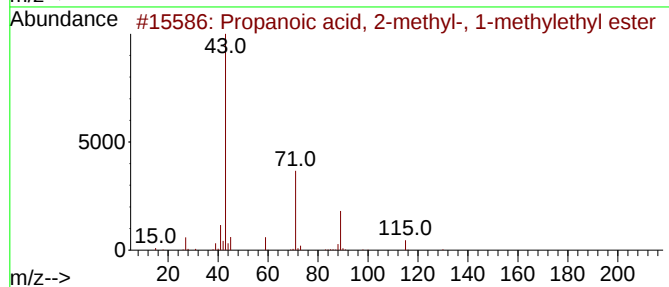
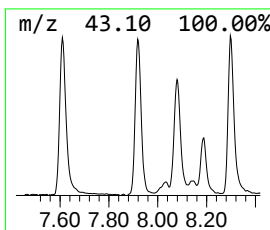
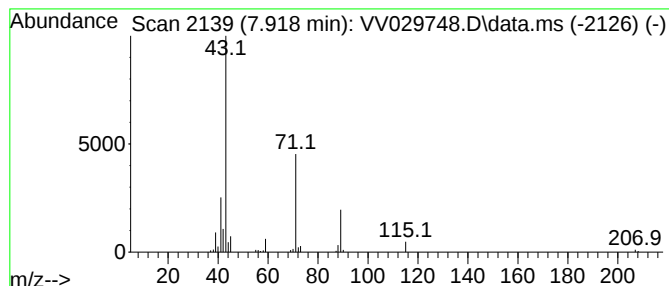
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.918	3.45 ug/L	91521	Chlorobenzene-d5	8.844

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
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	78
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122022\
Data File : VV029748.D
Acq On : 20 Dec 2022 14:00
Operator : SY/MD
Sample : PB149759TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB759

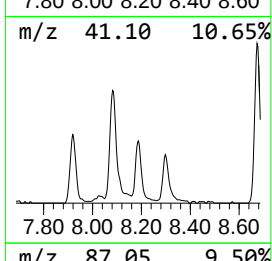
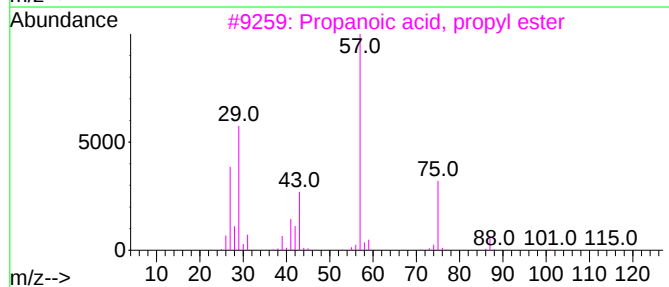
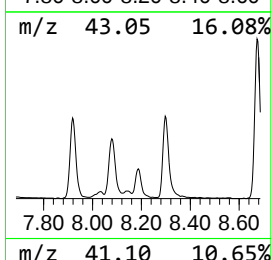
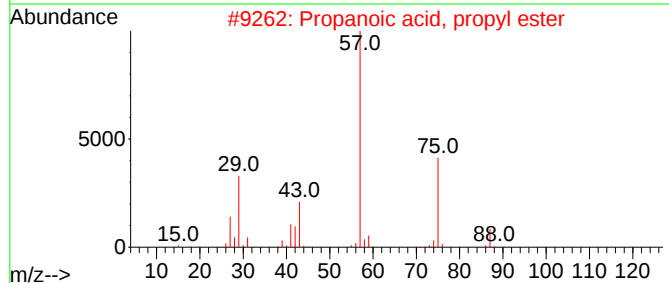
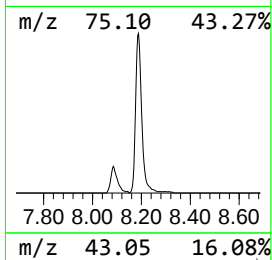
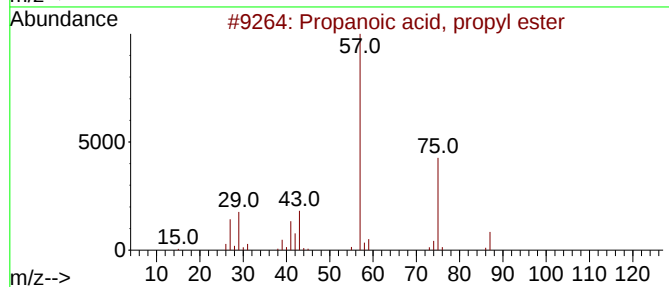
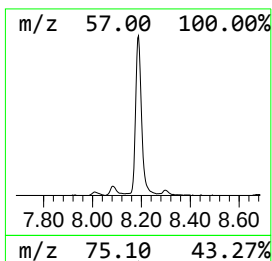
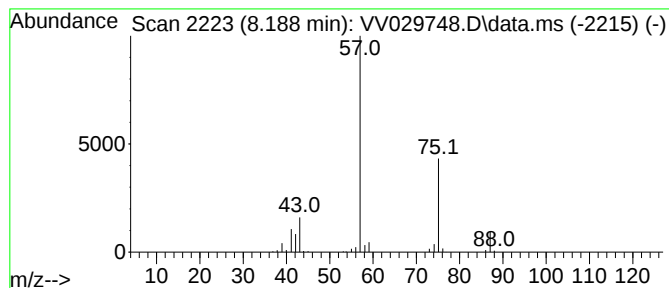
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.188	6.20 ug/L	164535	Chlorobenzene-d5	8.844

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, propyl ester	116	C6H12O2	000106-36-5	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122022\
Data File : VV029748.D
Acq On : 20 Dec 2022 14:00
Operator : SY/MD
Sample : PB149759TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB759

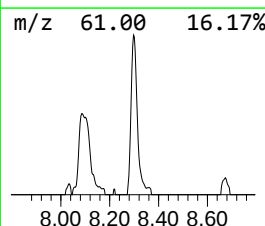
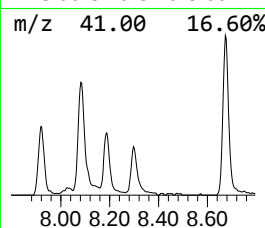
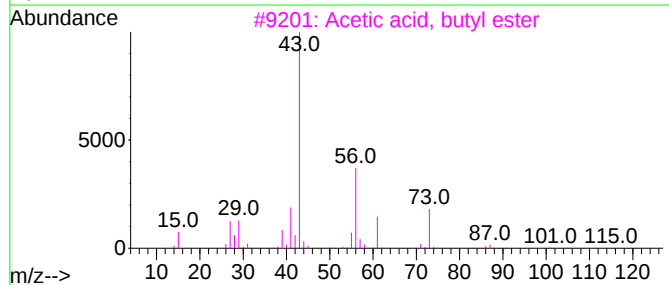
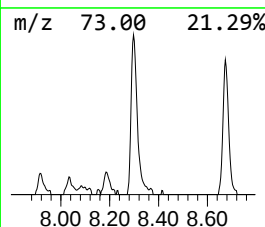
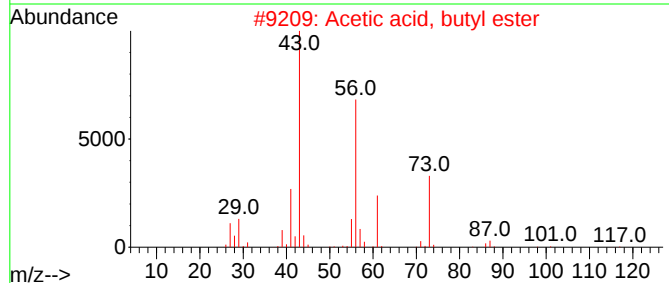
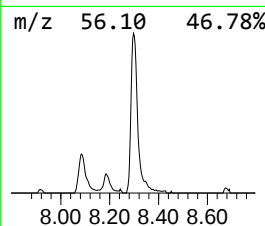
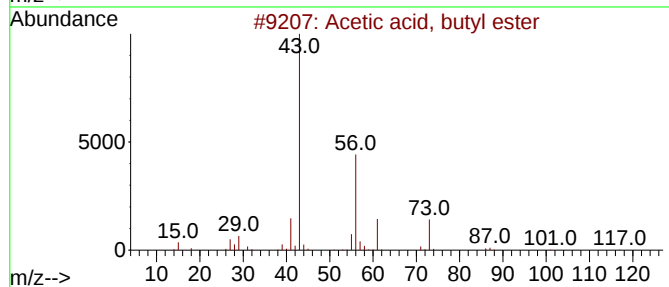
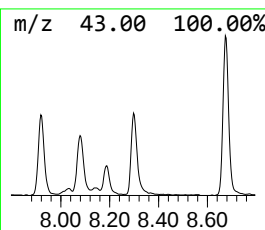
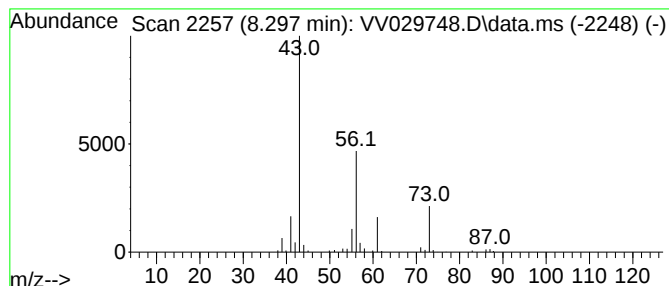
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.297	3.47 ug/L	92084	Chlorobenzene-d5	8.844

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	56
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	42
5			Isobutyl acetate	116	C6H12O2	000110-19-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122022\
Data File : VV029748.D
Acq On : 20 Dec 2022 14:00
Operator : SY/MD
Sample : PB149759TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB759

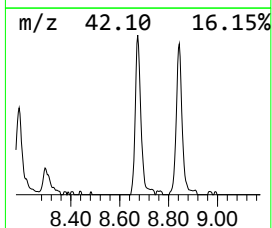
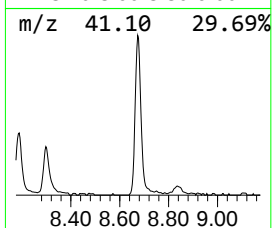
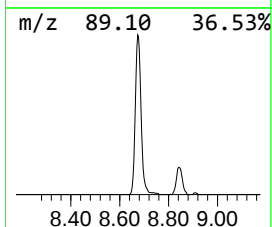
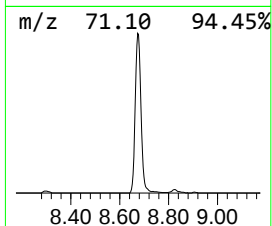
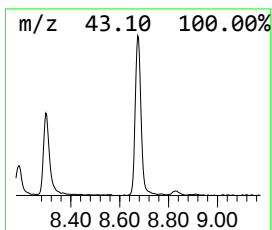
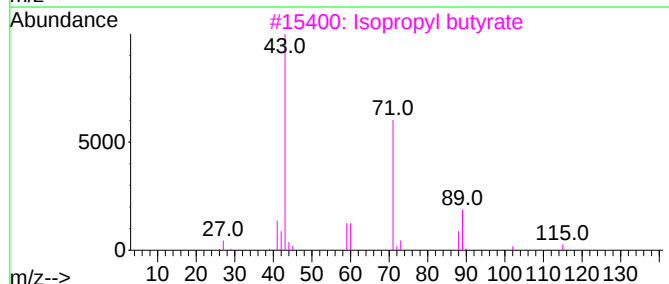
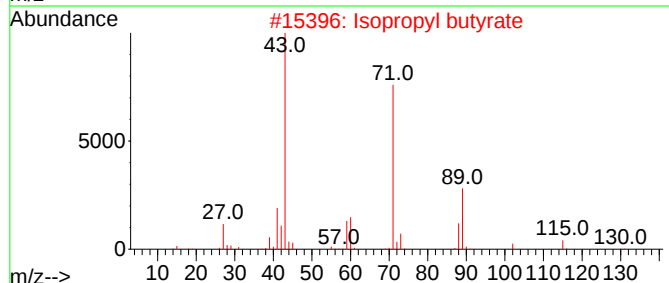
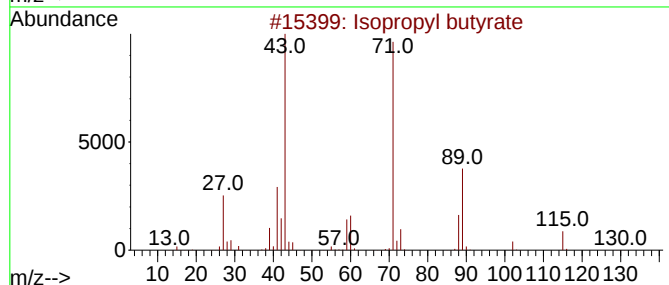
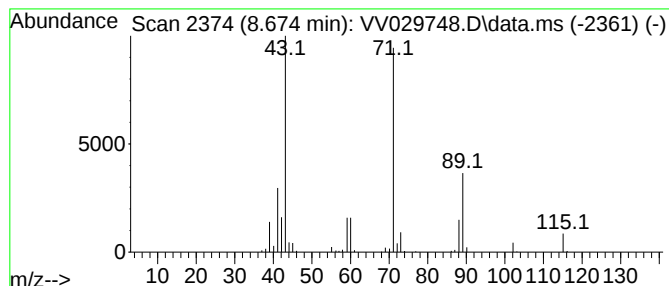
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Quant Title : VOC Analysis

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

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.674	9.87 ug/L	262070	Chlorobenzene-d5	8.844

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	72
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW122022\
Data File : VW029748.D
Acq On : 20 Dec 2022 14:00
Operator : SY/MD
Sample : PB149759TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB759

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.461	14.5	ug/L	314263	1	5.609	1086570	50.0
Propanoic acid,...	7.182	3.4	ug/L	74469	1	5.609	1086570	50.0
Propanoic acid,...	7.918	3.5	ug/L	91521	2	8.844	1327800	50.0
Propanoic acid,...	8.188	6.2	ug/L	164535	2	8.844	1327800	50.0
Acetic acid, bu...	8.297	3.5	ug/L	92084	2	8.844	1327800	50.0
Isopropyl butyrate	8.674	9.9	ug/L	262070	2	8.844	1327800	50.0