

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
 Data File : VV028017.D
 Acq On : 21 Sep 2022 15:30
 Operator : SY/MD
 Sample : N4689-02 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AY6

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: VV028017.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	74	80	97	rVB	169618	173626	14.52%	1.636%
2	1.555	153	160	172	rBV	141648	161207	13.49%	1.519%
3	2.098	318	329	342	rBV	303255	437418	36.59%	4.122%
4	2.272	379	383	386	rBV3	847	845	0.07%	0.008%
5	2.433	427	433	438	rVV5	751	883	0.07%	0.008%
6	2.497	444	453	464	rBV2	7427	11729	0.98%	0.111%
7	2.558	468	472	476	rVB3	433	405	0.03%	0.004%
8	2.610	480	488	489	rBV4	1749	2224	0.19%	0.021%
9	2.690	509	513	515	rBV2	558	412	0.03%	0.004%
10	3.175	661	664	666	rVV3	591	394	0.03%	0.004%
11	3.870	869	880	923	rBV2	122461	389899	32.62%	3.674%
12	4.336	1009	1025	1049	rBV	199820	487661	40.79%	4.595%
13	4.561	1090	1095	1099	rBV4	585	453	0.04%	0.004%
14	4.767	1155	1159	1163	rVB2	587	414	0.03%	0.004%
15	4.815	1168	1174	1177	rVB2	406	388	0.03%	0.004%
16	5.037	1226	1243	1273	rBV2	465174	1195413	100.00%	11.265%
17	5.285	1307	1320	1339	rBV3	8981	24770	2.07%	0.233%
18	5.410	1354	1359	1360	rBV3	957	749	0.06%	0.007%
19	5.548	1399	1402	1403	rBV3	1018	603	0.05%	0.006%
20	5.609	1408	1421	1438	rBV	396009	859940	71.94%	8.103%
21	6.063	1550	1562	1587	rVB	296789	608294	50.89%	5.732%
22	6.458	1676	1685	1709	rBV	113538	220459	18.44%	2.077%
23	6.982	1837	1848	1867	rVV	149670	273441	22.87%	2.577%
24	7.185	1900	1911	1925	rBV2	25379	45912	3.84%	0.433%
25	7.310	1937	1950	1969	rBV	563146	973046	81.40%	9.169%
26	7.616	2035	2045	2069	rBV	141332	250124	20.92%	2.357%
27	7.735	2080	2082	2086	rBV4	854	734	0.06%	0.007%
28	7.921	2130	2140	2152	rBV2	33465	58830	4.92%	0.554%
29	8.037	2167	2176	2180	rBV6	5661	8499	0.71%	0.080%
30	8.085	2181	2191	2215	rVV	437944	770549	64.46%	7.261%
31	8.191	2216	2224	2238	rVB	57884	96741	8.09%	0.912%
32	8.301	2250	2258	2281	rVB	34046	63123	5.28%	0.595%
33	8.677	2365	2375	2399	rBV2	90832	157241	13.15%	1.482%
34	8.847	2416	2428	2457	rBV	589675	954055	79.81%	8.990%
35	9.120	2510	2513	2516	rBV4	1487	1117	0.09%	0.011%
36	9.201	2536	2538	2541	rBV5	649	422	0.04%	0.004%

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37	9.310	2570	2572	2575	rBV2	646	416	0.03%	0.004%
38	9.394	2590	2598	2599	rBV7	1586	1938	0.16%	0.018%
39	9.548	2638	2646	2660	rBV4	7417	14322	1.20%	0.135%
40	9.719	2696	2699	2700	rBV3	733	410	0.03%	0.004%
41	9.747	2706	2708	2713	rVB3	508	374	0.03%	0.004%
42	9.879	2747	2749	2751	rBV2	757	396	0.03%	0.004%
43	9.934	2763	2766	2768	rVB2	739	387	0.03%	0.004%
44	10.005	2786	2788	2791	rBV2	936	688	0.06%	0.006%
45	10.030	2794	2796	2800	rVB4	656	471	0.04%	0.004%
46	10.053	2800	2803	2809	rBV2	633	747	0.06%	0.007%
47	10.117	2818	2823	2825	rBV4	1804	1541	0.13%	0.015%
48	10.156	2832	2835	2837	rBV2	760	392	0.03%	0.004%
49	10.214	2839	2853	2872	rBV	437101	686713	57.45%	6.471%
50	10.349	2893	2895	2900	rBV4	875	938	0.08%	0.009%
51	10.384	2903	2906	2914	rVB7	2014	2333	0.20%	0.022%
52	10.497	2937	2941	2942	rBV2	640	474	0.04%	0.004%
53	10.529	2948	2951	2952	rBV3	547	378	0.03%	0.004%
54	10.545	2954	2956	2962	rVB6	848	623	0.05%	0.006%
55	10.583	2962	2968	2976	rBV7	1135	1963	0.16%	0.018%
56	10.680	2995	2998	3001	rVV3	888	564	0.05%	0.005%
57	10.693	3001	3002	3006	rVB3	831	464	0.04%	0.004%
58	10.764	3022	3024	3027	rVB4	835	399	0.03%	0.004%
59	10.825	3041	3043	3046	rBV3	786	391	0.03%	0.004%
60	10.854	3050	3052	3056	rVB5	787	494	0.04%	0.005%
61	10.976	3086	3090	3091	rBV3	722	457	0.04%	0.004%
62	11.053	3112	3114	3118	rVB4	684	373	0.03%	0.004%
63	11.136	3137	3140	3142	rBV4	972	486	0.04%	0.005%
64	11.246	3162	3174	3194	rBV	516853	801127	67.02%	7.549%
65	11.387	3216	3218	3222	rVB4	1048	582	0.05%	0.005%
66	11.426	3226	3230	3231	rBV3	991	831	0.07%	0.008%
67	11.461	3238	3241	3246	rVB5	935	638	0.05%	0.006%
68	11.487	3246	3249	3251	rBV4	1088	576	0.05%	0.005%
69	11.622	3279	3291	3308	rBV	527539	835232	69.87%	7.870%
70	11.722	3320	3322	3326	rBV5	1182	783	0.07%	0.007%
71	11.792	3341	3344	3347	rBV5	1047	655	0.05%	0.006%
72	11.844	3357	3360	3362	rBV3	979	772	0.06%	0.007%
73	11.960	3393	3396	3400	rBV4	683	426	0.04%	0.004%
74	12.194	3466	3469	3474	rBV4	545	713	0.06%	0.007%
75	12.288	3496	3498	3505	rVB4	758	704	0.06%	0.007%
76	12.381	3525	3527	3532	rVB4	758	610	0.05%	0.006%

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 Title : VOC Analysis

77	12.480	3551	3558	3562	rVB5	1479	1876	0.16%	0.018%
78	12.509	3562	3567	3569	rBV4	1241	1099	0.09%	0.010%
79	12.654	3608	3612	3613	rBV2	1047	713	0.06%	0.007%
80	12.702	3624	3627	3631	rBV3	1036	719	0.06%	0.007%
81	12.921	3692	3695	3700	rVB6	979	773	0.06%	0.007%
82	13.008	3720	3722	3728	rVB5	642	466	0.04%	0.004%
83	13.095	3743	3749	3751	rBV3	735	735	0.06%	0.007%
84	13.214	3784	3786	3788	rBV3	764	455	0.04%	0.004%
85	13.349	3825	3828	3830	rBV3	833	472	0.04%	0.004%
86	13.509	3876	3878	3882	rBV4	1150	881	0.07%	0.008%
87	13.879	3991	3993	3996	rBV4	743	476	0.04%	0.004%
88	13.998	4024	4030	4032	rBV5	743	586	0.05%	0.006%
89	14.072	4049	4053	4054	rBV2	603	442	0.04%	0.004%
90	14.320	4127	4130	4133	rBV4	732	622	0.05%	0.006%
91	14.374	4144	4147	4149	rBV3	886	534	0.04%	0.005%
92	14.390	4149	4152	4154	rBV3	610	417	0.03%	0.004%
93	14.651	4229	4233	4236	rBV3	924	807	0.07%	0.008%
94	14.837	4287	4291	4293	rBV2	800	593	0.05%	0.006%
95	15.046	4354	4356	4358	rBV2	642	370	0.03%	0.003%
96	15.294	4430	4433	4439	rVB6	1214	1200	0.10%	0.011%
97	15.439	4476	4478	4482	rBV5	902	594	0.05%	0.006%
98	15.538	4507	4509	4513	rBV5	695	550	0.05%	0.005%
99	15.712	4560	4563	4566	rBV3	944	763	0.06%	0.007%
100	15.950	4635	4637	4641	rBV6	1771	1260	0.11%	0.012%

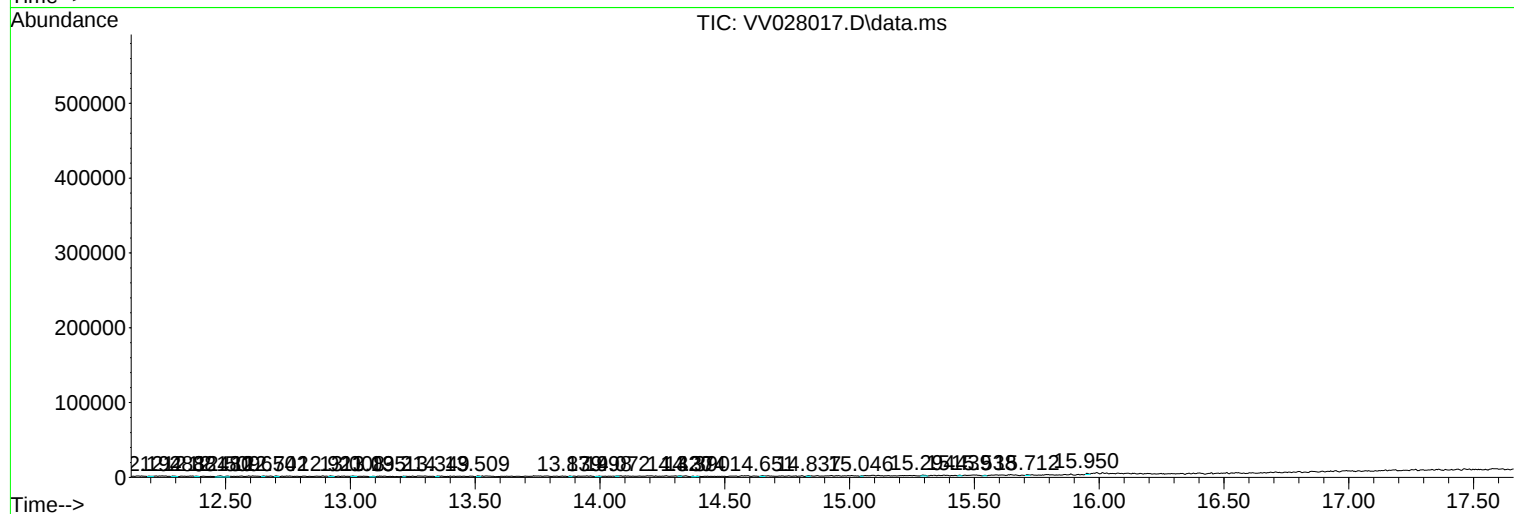
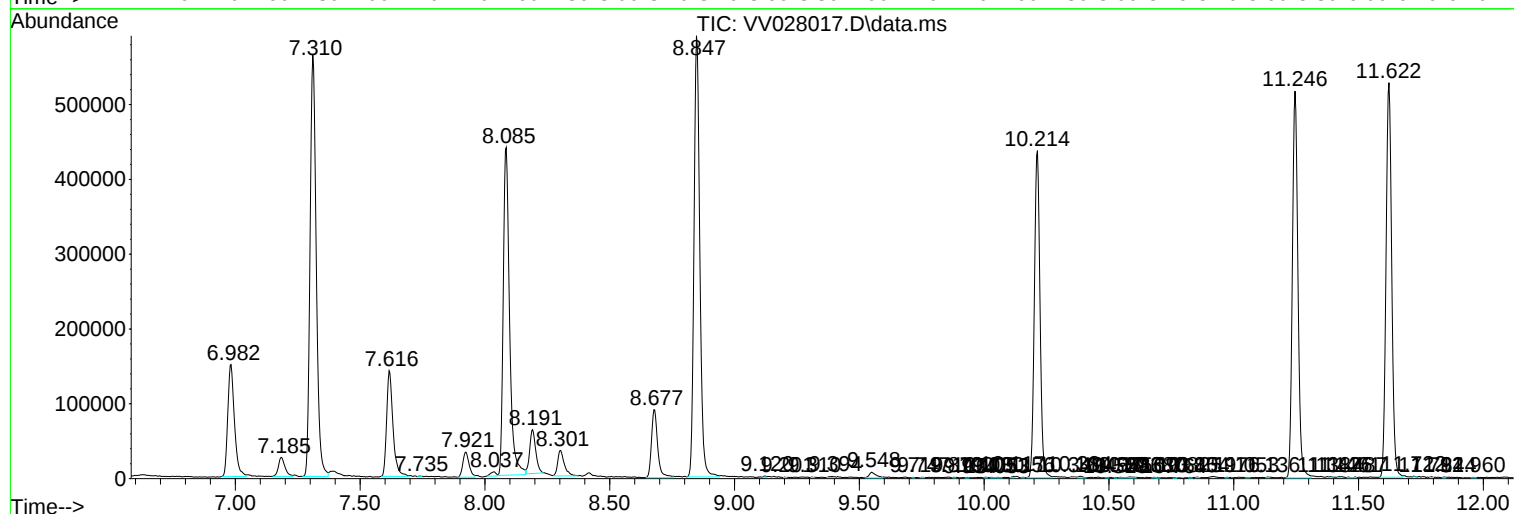
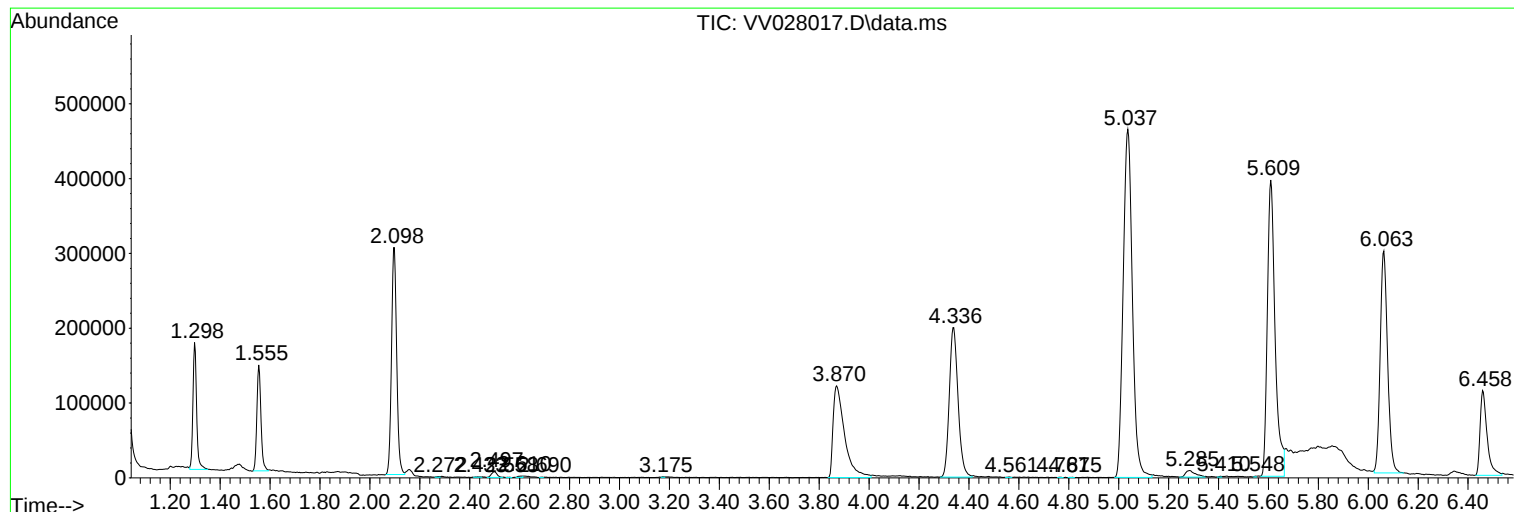
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Instrument :
MSVOA_V
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

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



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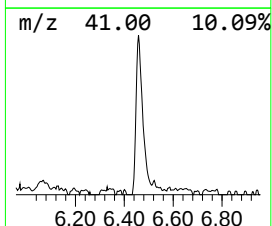
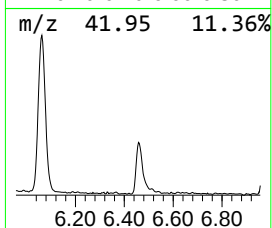
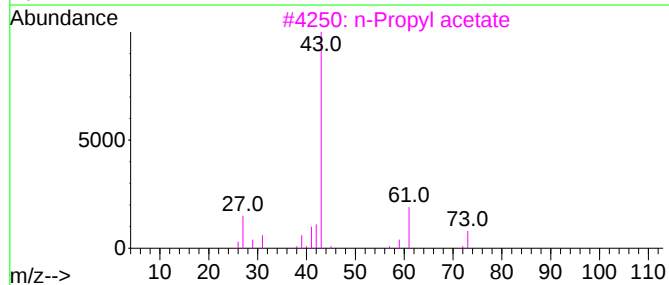
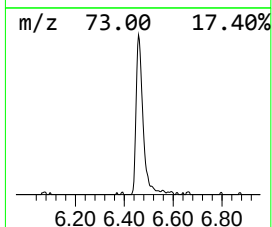
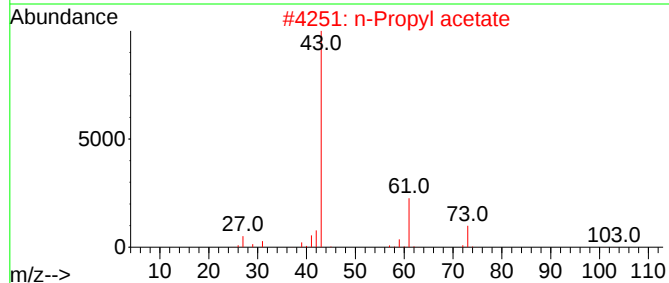
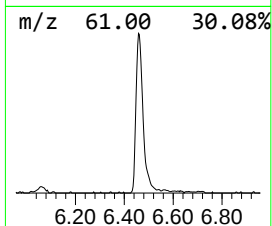
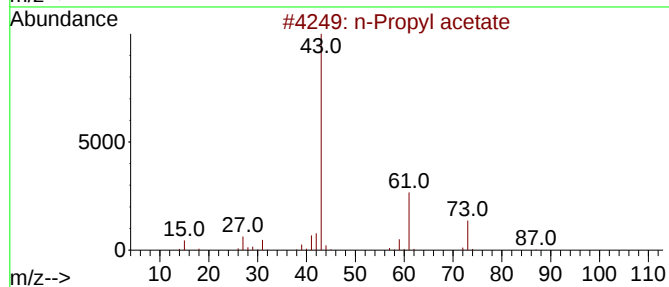
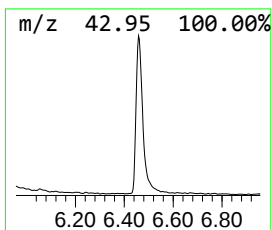
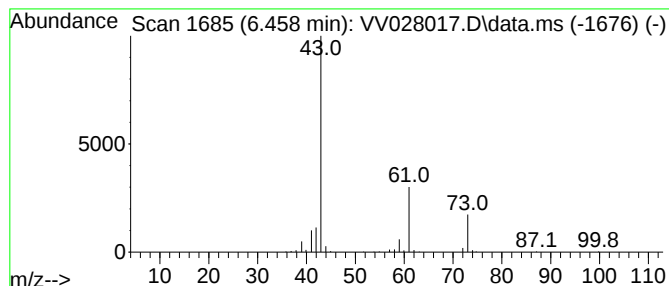
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

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	12.82 ug/L	220459	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	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	72
4	Isopropyl acetate			102	C5H10O2	000108-21-4	36
5	Propanal, 2,3-dihydroxy-, (S)-			90	C3H6O3	000497-09-6	36



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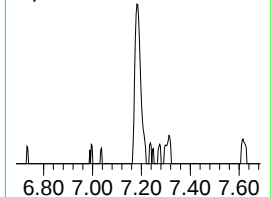
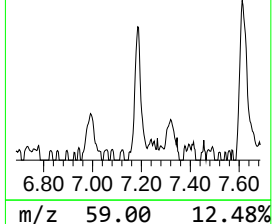
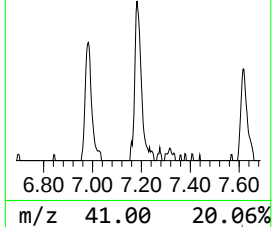
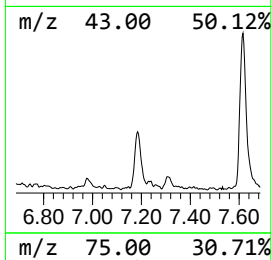
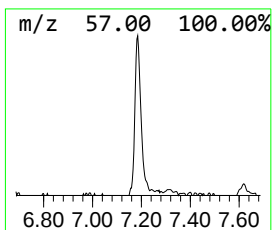
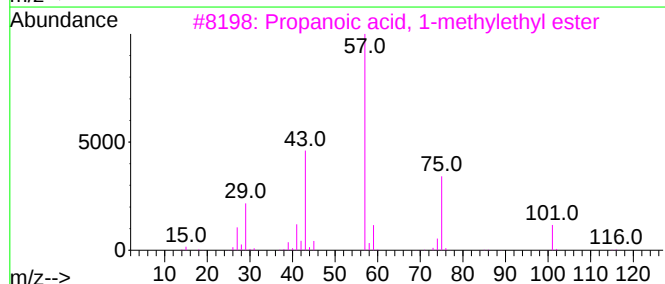
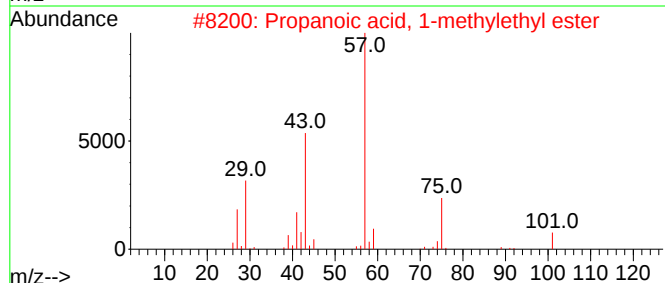
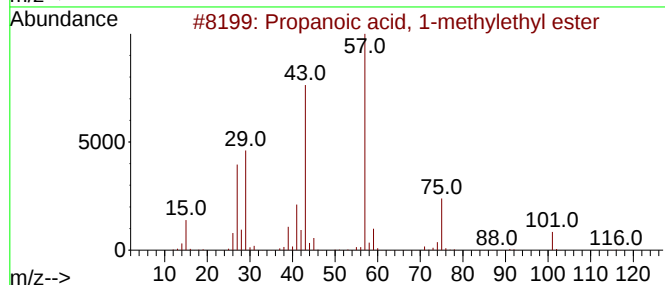
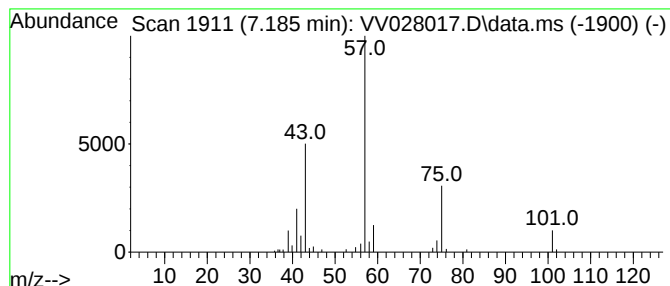
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.185	2.67 ug/L	45912	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	78
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	40



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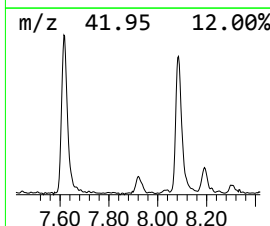
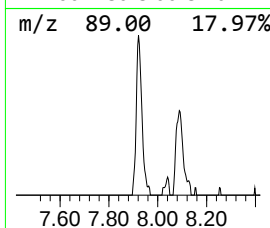
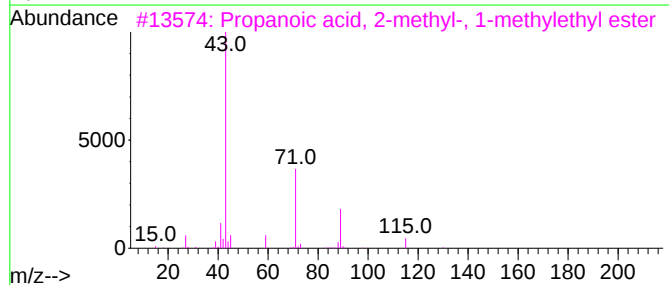
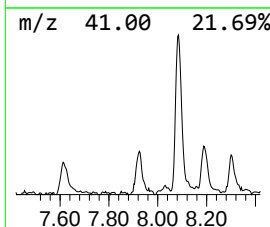
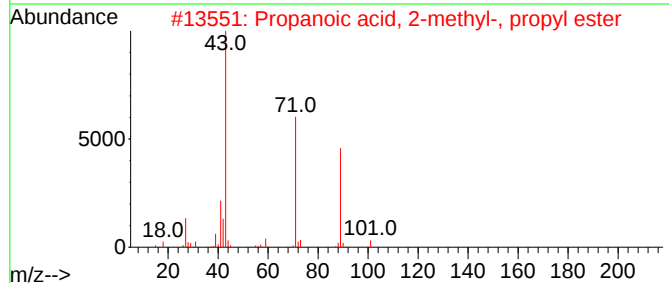
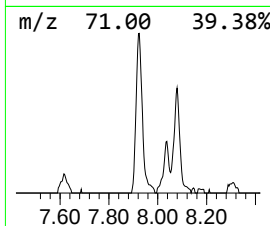
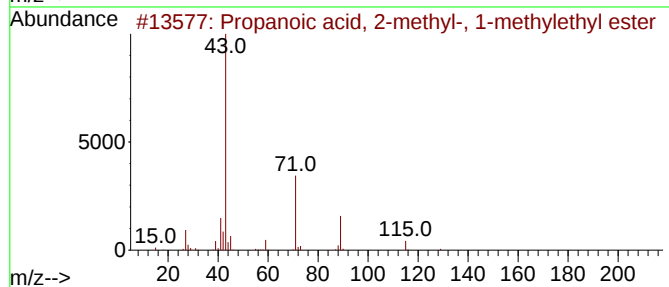
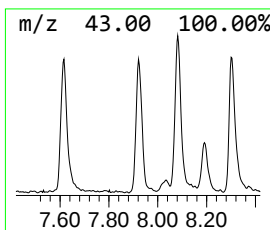
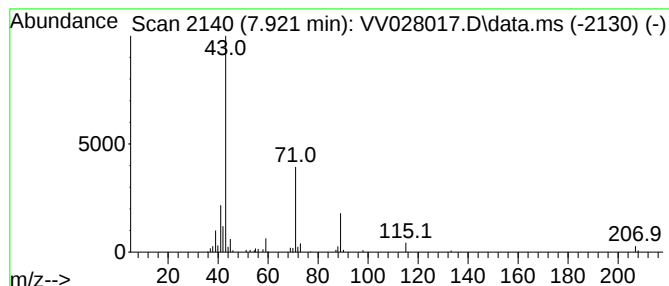
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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.921	3.08 ug/L	58830	Chlorobenzene-d5	8.847

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-, propy...	130	C7H14O2	000644-49-5	72
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
4			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	64
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028017.D
Acq On : 21 Sep 2022 15:30
Operator : SY/MD
Sample : N4689-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY6

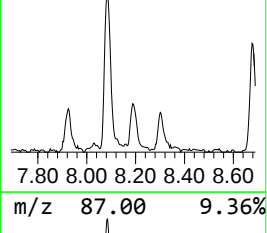
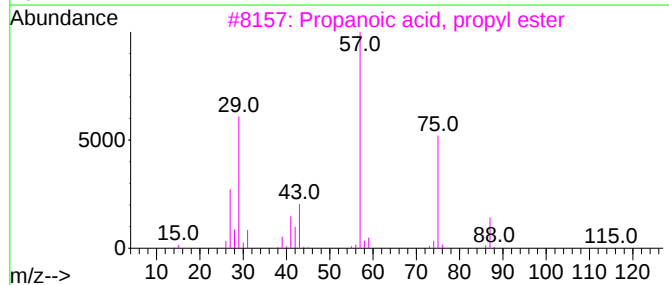
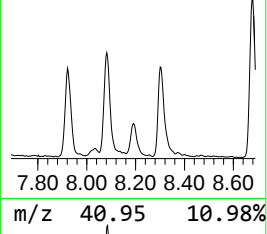
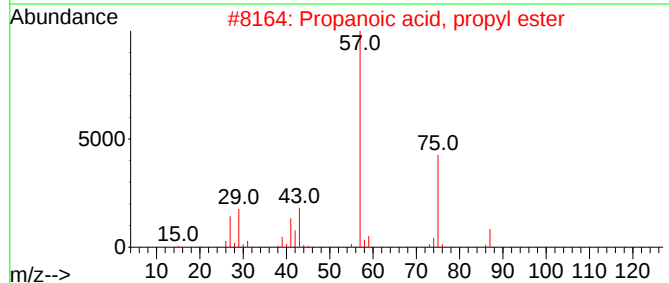
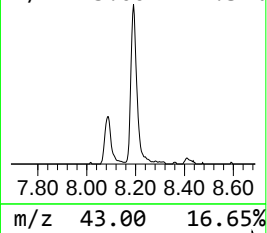
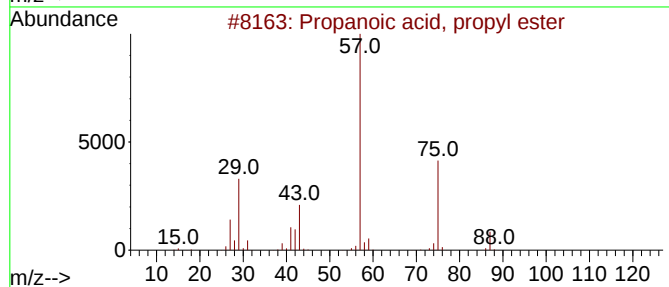
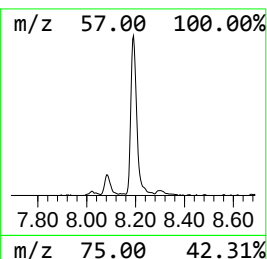
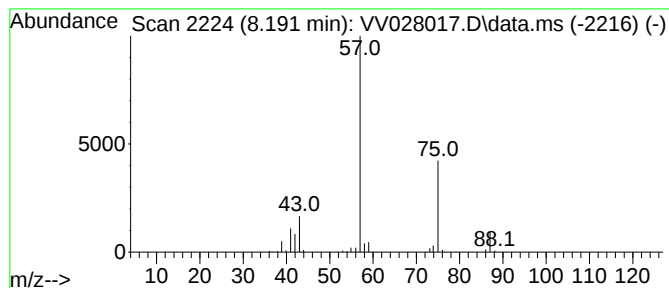
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.191	5.07 ug/L	96741	Chlorobenzene-d5	8.847

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	74
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028017.D
Acq On : 21 Sep 2022 15:30
Operator : SY/MD
Sample : N4689-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY6

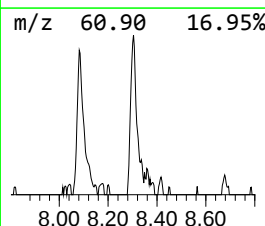
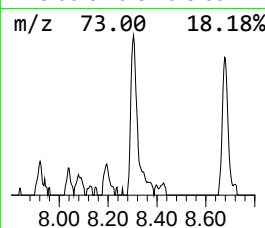
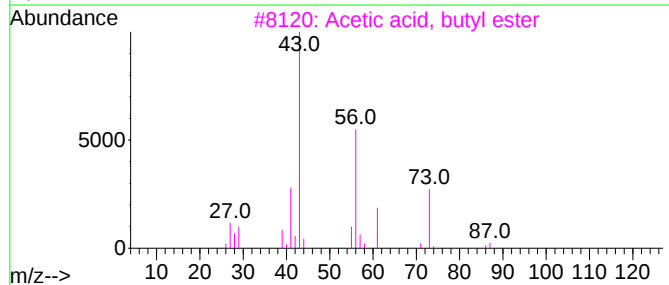
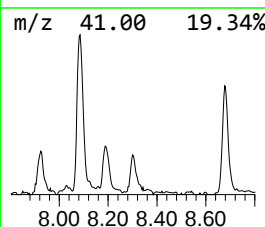
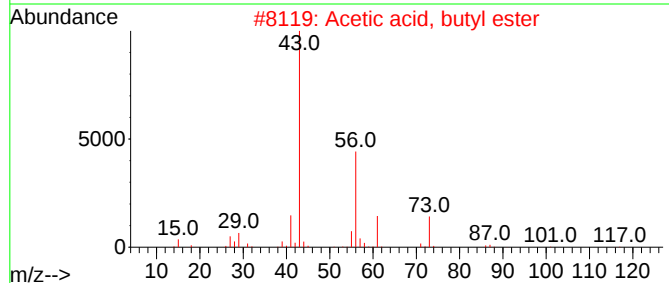
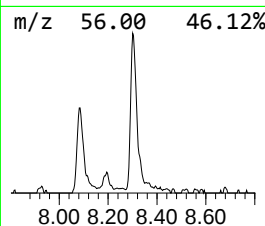
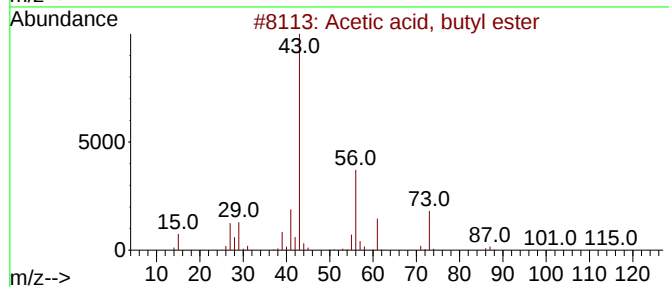
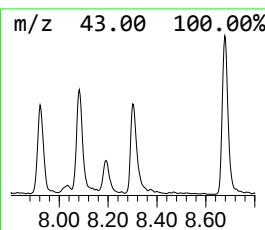
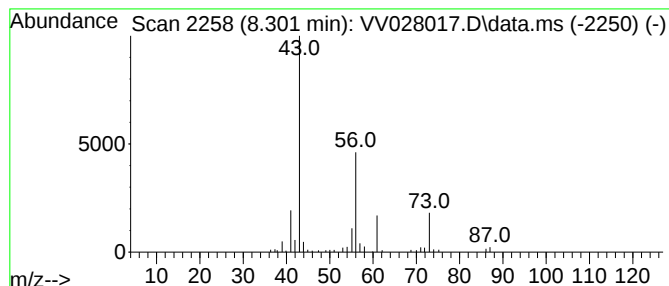
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.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.
8.301	3.31 ug/L	63123	Chlorobenzene-d5	8.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
5			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028017.D
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Operator : SY/MD
Sample : N4689-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY6

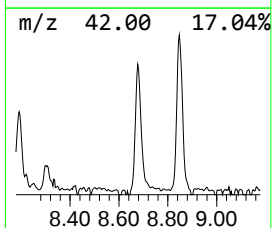
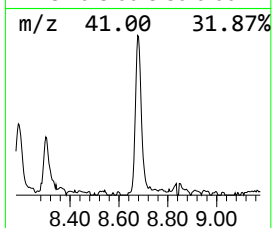
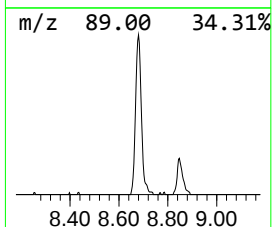
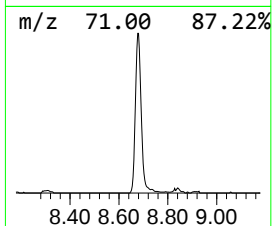
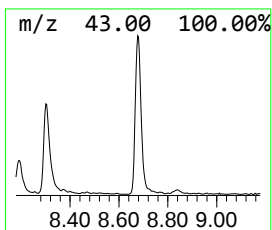
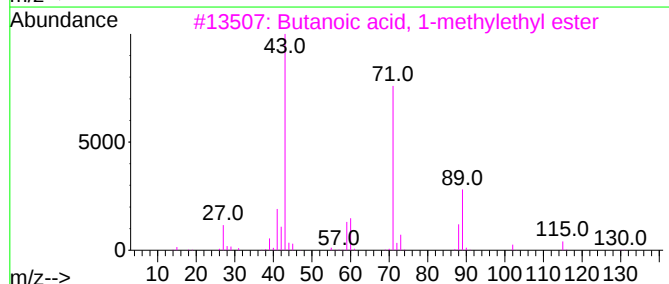
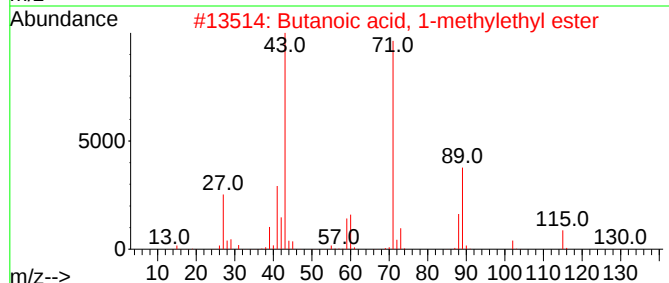
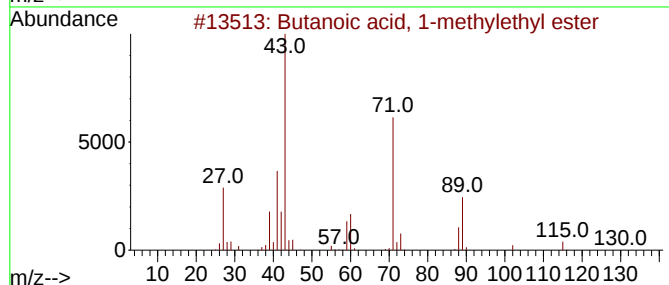
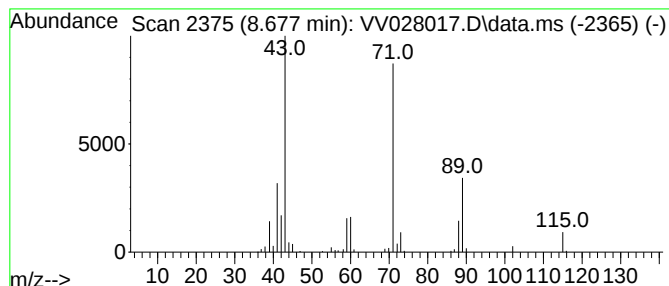
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Quant Title : VOC Analysis

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

Peak Number 7 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.677	8.24 ug/L	157241	Chlorobenzene-d5	8.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
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			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	78
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY6

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	12.8	ug/L	220459	1	5.609	859940	50.0
Propanoic acid,...	7.185	2.7	ug/L	45912	1	5.609	859940	50.0
Propanoic acid,...	7.921	3.1	ug/L	58830	2	8.847	954055	50.0
Propanoic acid,...	8.191	5.1	ug/L	96741	2	8.847	954055	50.0
Acetic acid, bu...	8.301	3.3	ug/L	63123	2	8.847	954055	50.0
Butanoic acid, ...	8.677	8.2	ug/L	157241	2	8.847	954055	50.0