

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW121922\
 Data File : VW029719.D
 Acq On : 19 Dec 2022 14:16
 Operator : SY/MD
 Sample : N6075-09 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGSM5

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: VW029719.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	76	82	98	rVB	213820	216545	14.71%	1.685%
2	1.555	155	160	178	rVB	160039	184473	12.53%	1.435%
3	2.102	319	330	343	rBV	358173	509836	34.63%	3.967%
4	2.500	445	454	467	rVB	9837	16249	1.10%	0.126%
5	2.616	478	490	501	rBV2	4854	9590	0.65%	0.075%
6	2.728	521	525	529	rVB2	207	145	0.01%	0.001%
7	2.754	529	533	534	rBV	282	188	0.01%	0.001%
8	2.847	559	562	566	rBV2	250	177	0.01%	0.001%
9	2.902	577	579	584	rVB2	311	222	0.02%	0.002%
10	2.950	591	594	599	rVB	235	165	0.01%	0.001%
11	3.008	609	612	616	rVB2	127	114	0.01%	0.001%
12	3.037	616	621	624	rBV2	245	254	0.02%	0.002%
13	3.185	658	667	671	rBV3	861	1371	0.09%	0.011%
14	3.301	700	703	705	rBV	147	93	0.01%	0.001%
15	3.462	749	753	757	rBV2	194	157	0.01%	0.001%
16	3.487	758	761	769	rVB2	171	204	0.01%	0.002%
17	3.587	789	792	794	rBV	173	105	0.01%	0.001%
18	3.651	810	812	815	rVB	222	97	0.01%	0.001%
19	3.732	835	837	841	rVB2	248	115	0.01%	0.001%
20	3.825	863	866	871	rBV2	174	159	0.01%	0.001%
21	3.876	871	882	926	rBV	96785	309437	21.02%	2.408%
22	4.336	1009	1025	1055	rBV	227788	566890	38.50%	4.411%
23	4.590	1103	1104	1107	rVB2	191	101	0.01%	0.001%
24	4.619	1111	1113	1114	rBV	173	89	0.01%	0.001%
25	4.671	1126	1129	1132	rVB3	180	103	0.01%	0.001%
26	4.732	1143	1148	1153	rBV2	167	166	0.01%	0.001%
27	4.783	1162	1164	1167	rBV	210	94	0.01%	0.001%
28	4.825	1174	1177	1181	rVB2	202	159	0.01%	0.001%
29	4.854	1181	1186	1189	rBV2	105	111	0.01%	0.001%
30	4.880	1189	1194	1196	rBV	171	110	0.01%	0.001%
31	4.937	1209	1212	1216	rBV	158	96	0.01%	0.001%
32	4.976	1216	1224	1226	rBV2	127	100	0.01%	0.001%
33	5.037	1226	1243	1269	rBV2	571667	1472305	100.00%	11.455%
34	5.285	1311	1320	1343	rVB3	11014	26519	1.80%	0.206%
35	5.519	1391	1393	1395	rVB	218	91	0.01%	0.001%
36	5.558	1395	1405	1408	rBV3	338	476	0.03%	0.004%

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Integrator: RTE

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

37	5.609	1408	1421	1452	rBV	517847	1051339	71.41%	8.180%
38	5.851	1494	1496	1502	rVB3	433	327	0.02%	0.003%
39	5.899	1502	1511	1523	rBV5	5280	10619	0.72%	0.083%
40	5.992	1532	1540	1543	rBV4	898	1124	0.08%	0.009%
41	6.060	1548	1561	1594	rBV	314953	657667	44.67%	5.117%
42	6.288	1630	1632	1634	rVB2	299	144	0.01%	0.001%
43	6.304	1634	1637	1640	rBV2	315	163	0.01%	0.001%
44	6.352	1640	1652	1667	rBV2	4663	13030	0.89%	0.101%
45	6.461	1676	1686	1715	rBV	138446	270314	18.36%	2.103%
46	6.796	1786	1790	1797	rVB2	457	469	0.03%	0.004%
47	6.857	1805	1809	1811	rBV3	296	214	0.01%	0.002%
48	6.979	1835	1847	1877	rBV	165682	306595	20.82%	2.385%
49	7.182	1900	1910	1922	rBV2	32128	56628	3.85%	0.441%
50	7.307	1937	1949	1979	rBV	697443	1229538	83.51%	9.566%
51	7.613	2033	2044	2063	rBV2	155261	273121	18.55%	2.125%
52	7.918	2126	2139	2157	rBV	42659	74596	5.07%	0.580%
53	8.034	2162	2175	2180	rBV8	7968	14445	0.98%	0.112%
54	8.085	2181	2191	2214	rVV	353065	669232	45.45%	5.207%
55	8.188	2217	2223	2246	rVV	73757	125784	8.54%	0.979%
56	8.301	2249	2258	2275	rBV	42149	71842	4.88%	0.559%
57	8.535	2328	2331	2333	rBV3	499	356	0.02%	0.003%
58	8.596	2348	2350	2355	rVB3	372	310	0.02%	0.002%
59	8.674	2361	2374	2396	rBV	127845	207766	14.11%	1.617%
60	8.789	2408	2410	2414	rBV3	468	297	0.02%	0.002%
61	8.844	2414	2427	2456	rBV	777728	1273703	86.51%	9.910%
62	9.111	2502	2510	2514	rBV5	1776	2355	0.16%	0.018%
63	9.182	2529	2532	2535	rVB3	373	182	0.01%	0.001%
64	9.236	2546	2549	2554	rVB2	312	227	0.02%	0.002%
65	9.278	2558	2562	2566	rVV	204	158	0.01%	0.001%
66	9.326	2574	2577	2580	rBV	157	120	0.01%	0.001%
67	9.387	2588	2596	2604	rBV3	1505	2277	0.15%	0.018%
68	9.465	2615	2620	2626	rBV2	124	161	0.01%	0.001%
69	9.542	2635	2644	2657	rBV2	10212	16956	1.15%	0.132%
70	9.731	2700	2703	2704	rBV	185	88	0.01%	0.001%
71	9.921	2755	2762	2763	rBV3	319	336	0.02%	0.003%
72	10.005	2785	2788	2789	rBV	231	120	0.01%	0.001%
73	10.030	2793	2796	2801	rVV2	145	108	0.01%	0.001%
74	10.162	2827	2837	2841	rBV	16145	24191	1.64%	0.188%
75	10.207	2842	2851	2873	rVB	465297	730424	49.61%	5.683%
76	10.371	2895	2902	2912	rVB5	1518	2396	0.16%	0.019%

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 Title : VOC Analysis

77	10.510	2942	2945	2946	rBV5	174	87	0.01%	0.001%
78	10.522	2946	2949	2954	rVV2	391	397	0.03%	0.003%
79	10.567	2956	2963	2976	rVB	8322	12892	0.88%	0.100%
80	10.696	3000	3003	3008	rBV	309	290	0.02%	0.002%
81	10.722	3009	3011	3015	rVB	266	124	0.01%	0.001%
82	10.741	3015	3017	3021	rVB2	268	148	0.01%	0.001%
83	10.760	3021	3023	3025	rBV2	258	110	0.01%	0.001%
84	10.818	3038	3041	3045	rBV3	231	195	0.01%	0.002%
85	11.059	3113	3116	3120	rVB2	249	187	0.01%	0.001%
86	11.079	3120	3122	3123	rBV	202	88	0.01%	0.001%
87	11.092	3124	3126	3130	rVB2	339	214	0.01%	0.002%
88	11.236	3159	3171	3194	rBV	835429	1295012	87.96%	10.076%
89	11.535	3263	3264	3268	rVB3	304	174	0.01%	0.001%
90	11.612	3276	3288	3317	rBV	718014	1132573	76.93%	8.812%
91	11.854	3361	3363	3366	rBV2	315	187	0.01%	0.001%
92	11.969	3396	3399	3401	rBV	186	89	0.01%	0.001%
93	11.985	3402	3404	3408	rVV	360	223	0.02%	0.002%
94	12.018	3412	3414	3420	rVV3	360	266	0.02%	0.002%
95	12.085	3433	3435	3438	rBV2	408	188	0.01%	0.001%
96	12.153	3451	3456	3457	rBV	332	264	0.02%	0.002%
97	12.239	3476	3483	3485	rBV3	1335	1579	0.11%	0.012%
98	12.400	3530	3533	3534	rBV2	377	209	0.01%	0.002%
99	12.519	3568	3570	3575	rVB3	482	249	0.02%	0.002%
100	12.667	3612	3616	3617	rBV	247	176	0.01%	0.001%

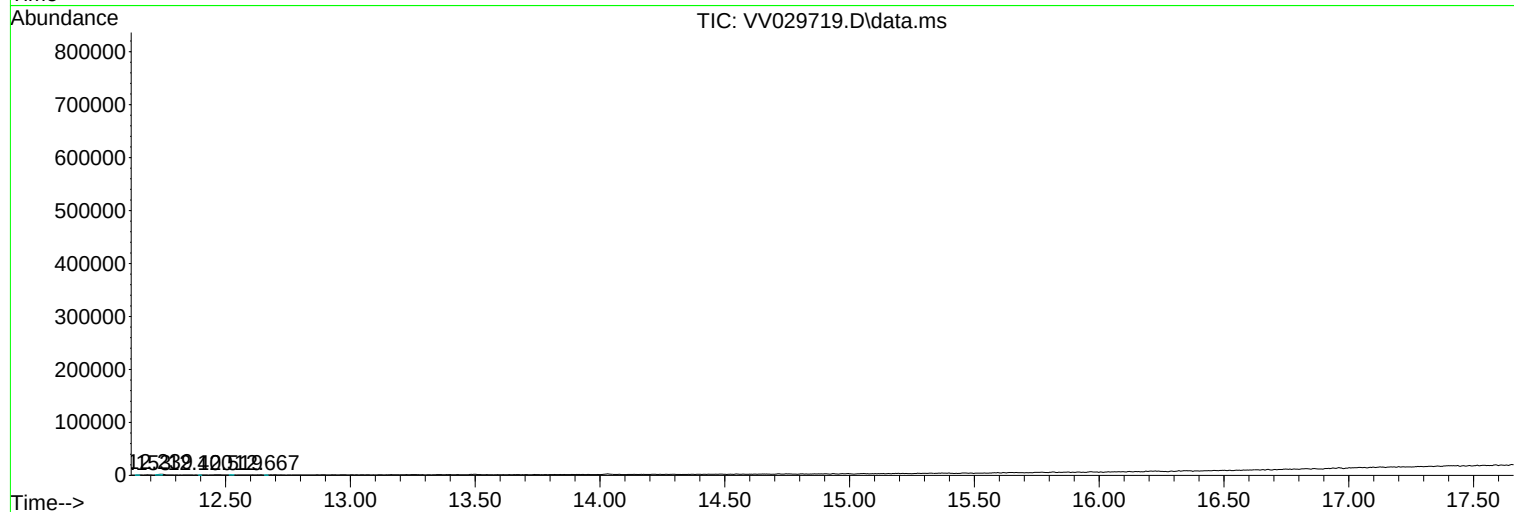
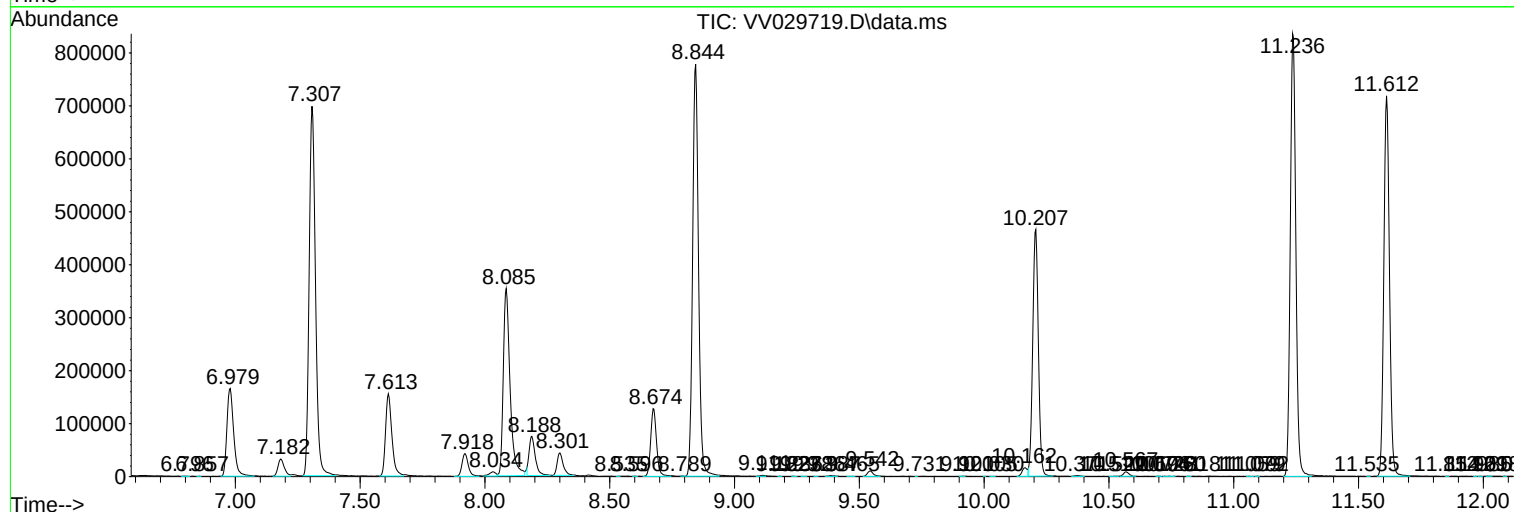
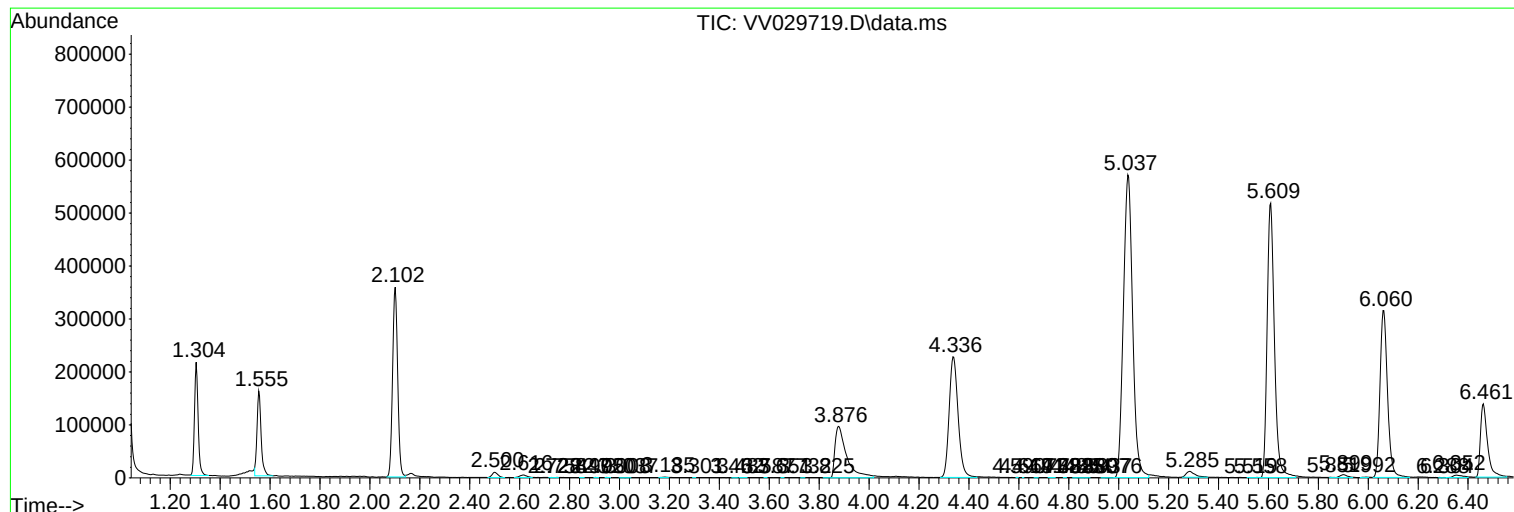
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029719.D
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Operator : SY/MD
Sample : N6075-09 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM5

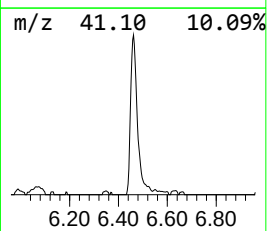
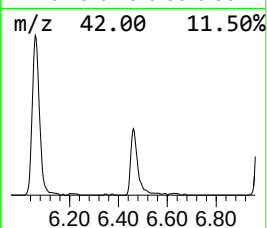
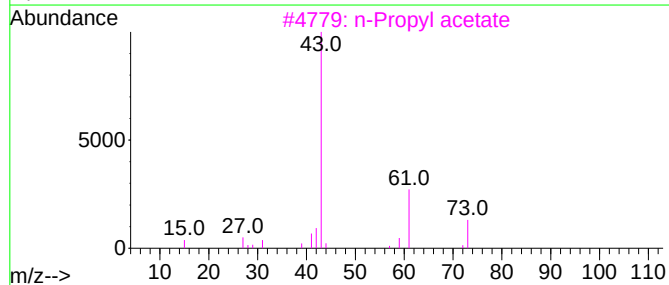
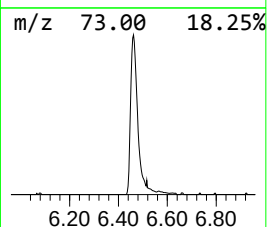
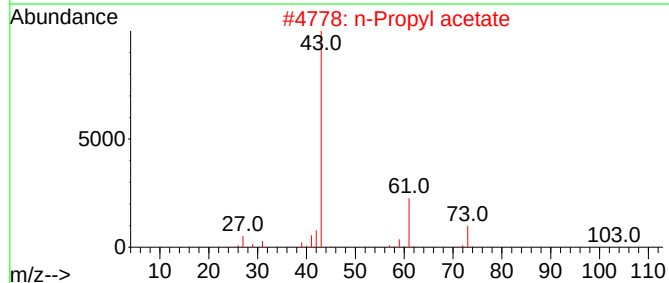
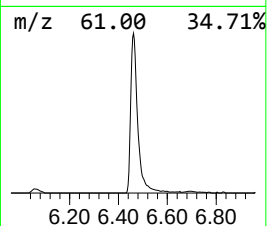
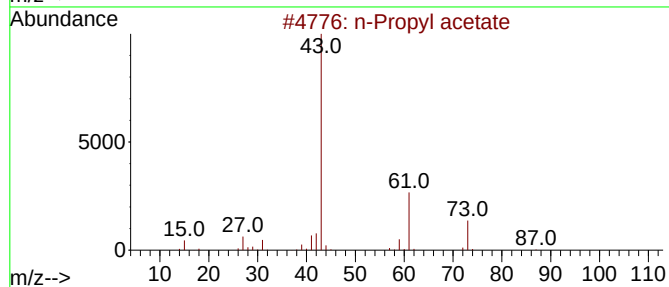
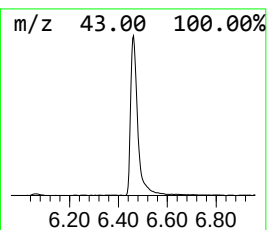
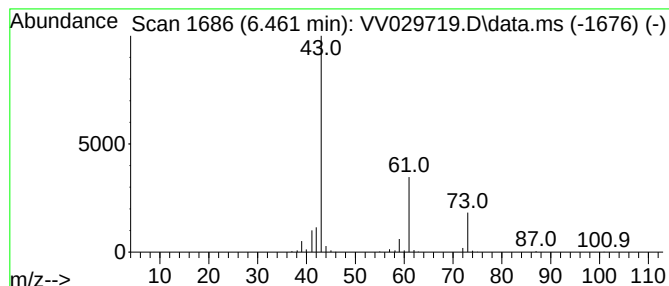
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.461	12.86 ug/L	270314	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	64
5	Propanal, 2,3-dihydroxy-, (S)-			90	C3H6O3	000497-09-6	36



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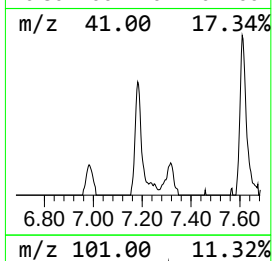
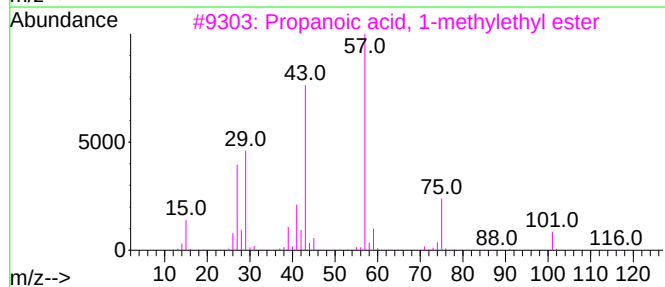
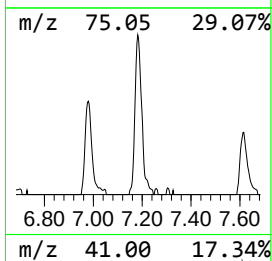
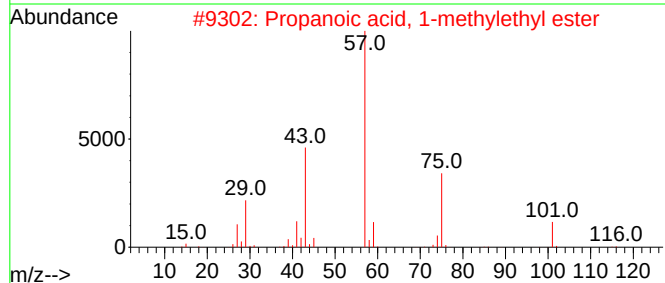
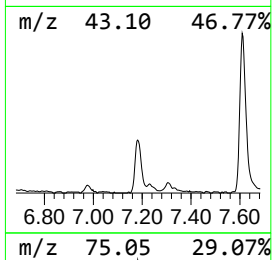
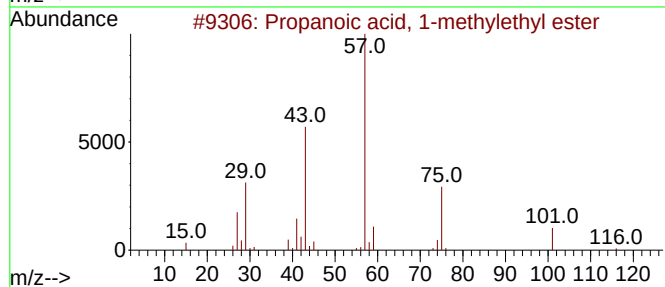
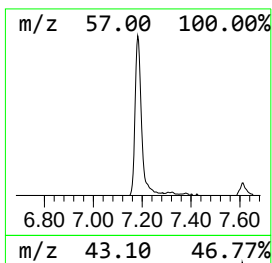
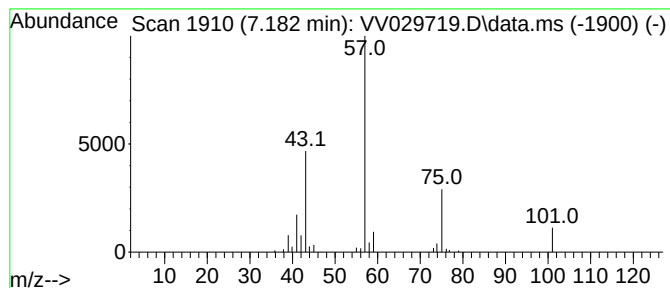
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.182	2.69 ug/L	56628	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	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45



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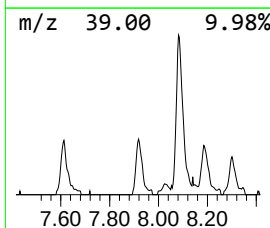
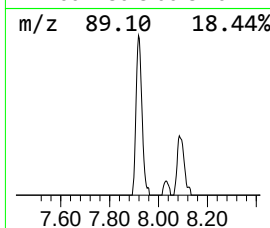
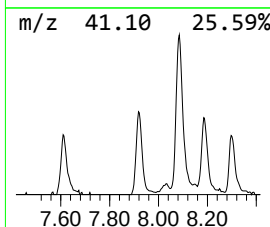
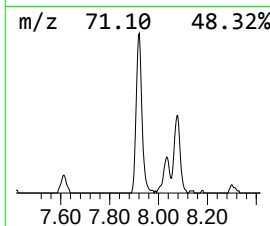
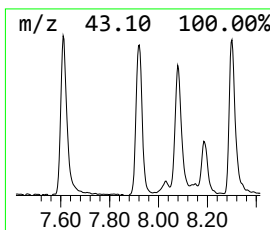
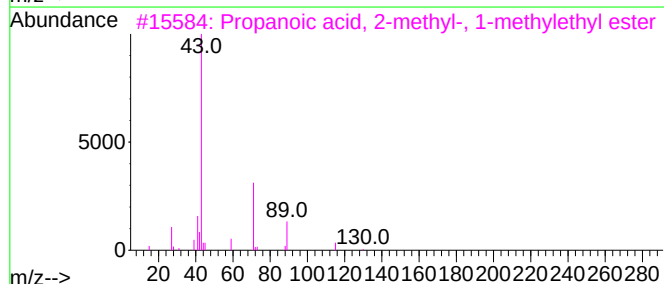
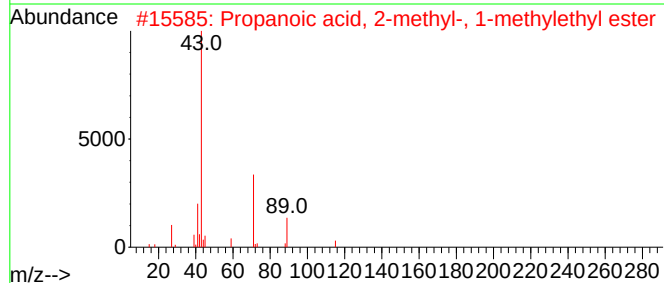
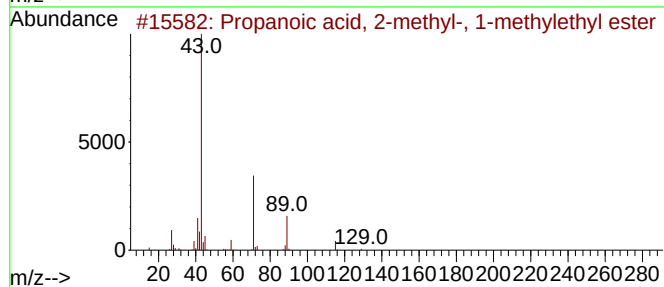
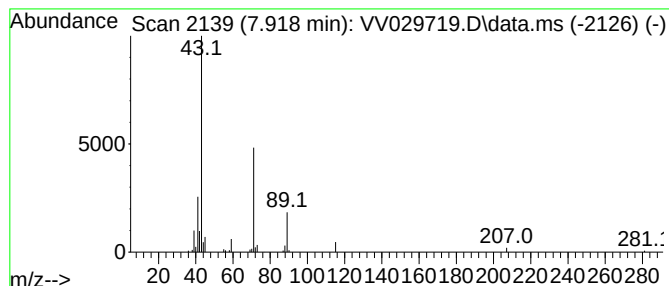
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.918	2.93 ug/L	74596	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	83
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
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\VV121922\
Data File : VV029719.D
Acq On : 19 Dec 2022 14:16
Operator : SY/MD
Sample : N6075-09 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM5

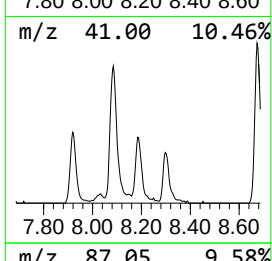
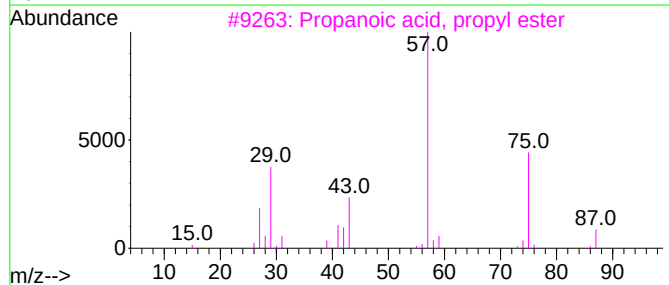
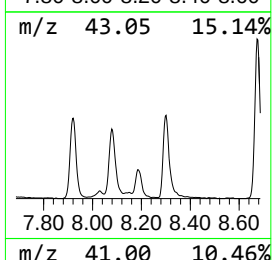
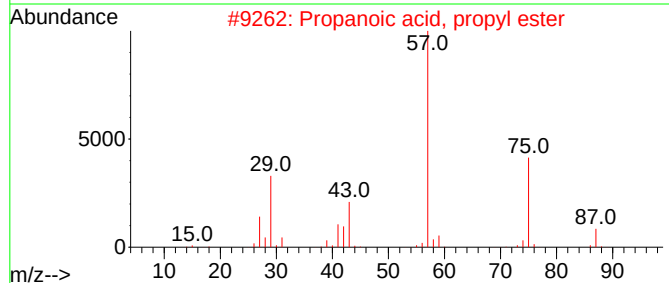
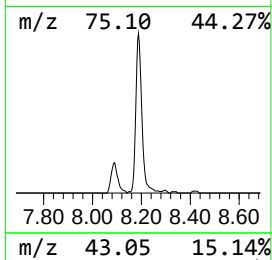
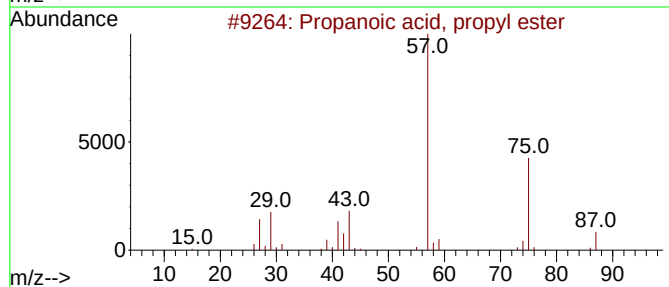
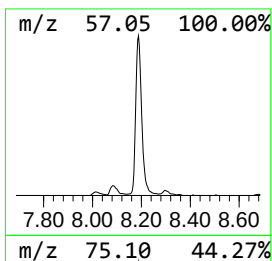
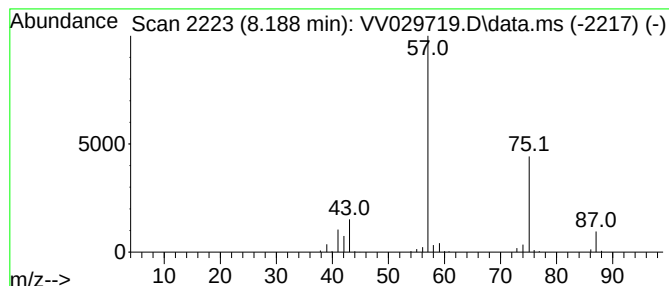
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Quant Title : VOC Analysis

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	4.94 ug/L	125784	Chlorobenzene-d5	8.844

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	47
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	45
5			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029719.D
Acq On : 19 Dec 2022 14:16
Operator : SY/MD
Sample : N6075-09 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM5

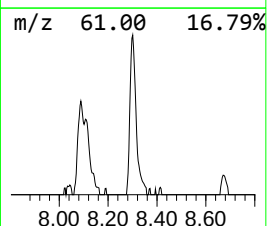
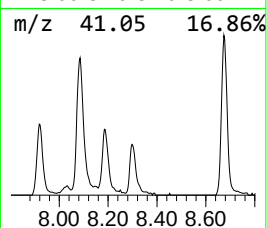
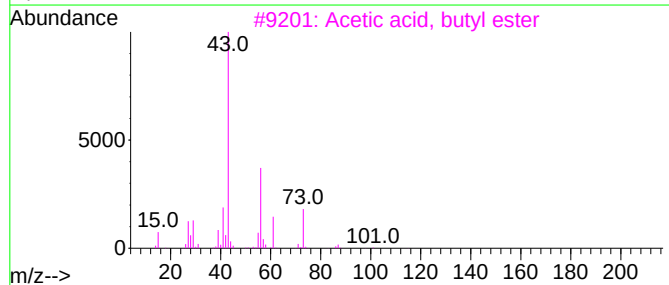
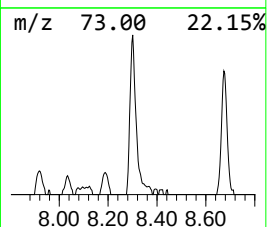
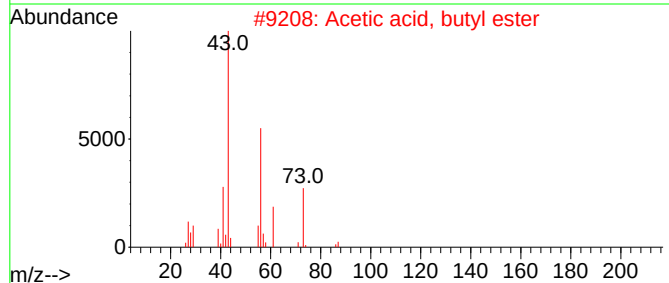
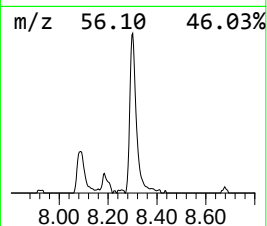
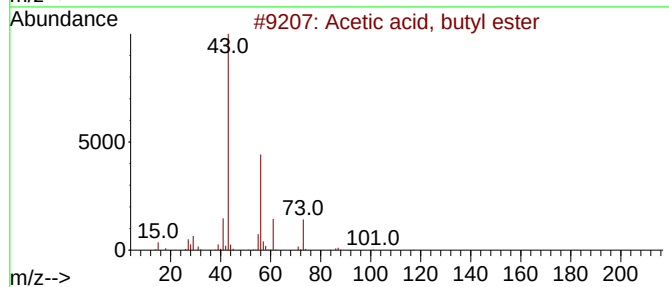
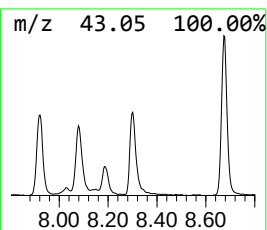
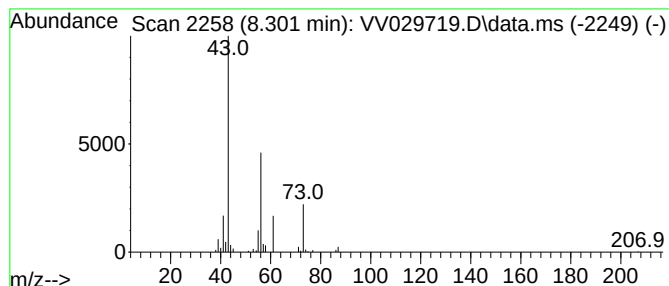
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.301	2.82 ug/L	71842	Chlorobenzene-d5	8.844

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	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\VV121922\
Data File : VV029719.D
Acq On : 19 Dec 2022 14:16
Operator : SY/MD
Sample : N6075-09 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM5

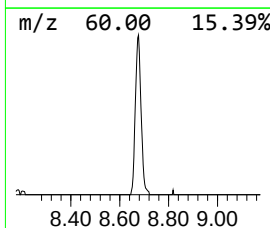
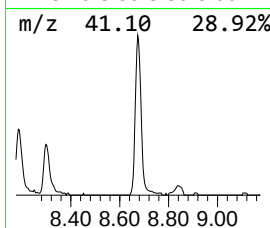
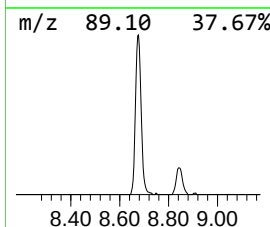
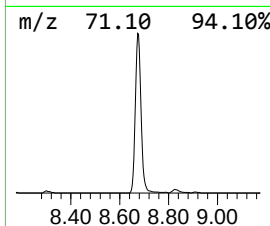
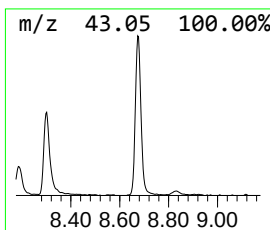
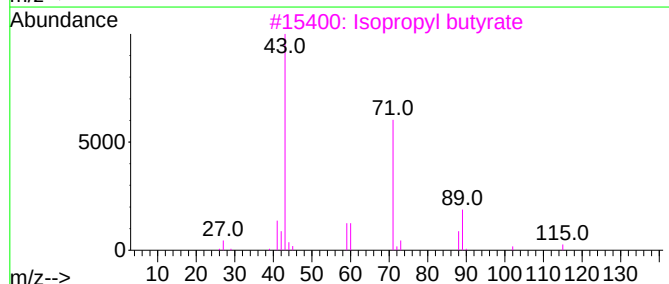
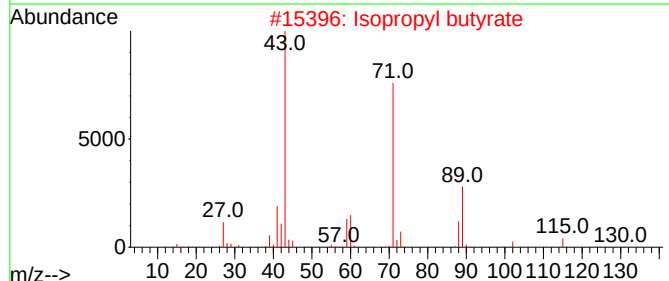
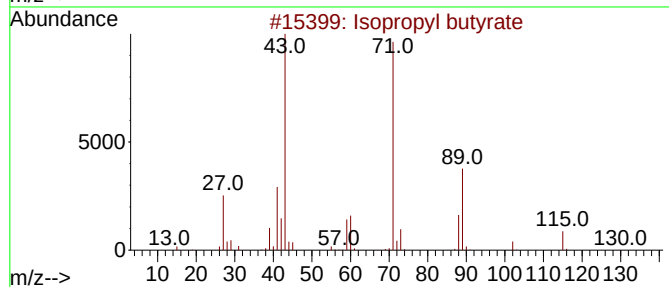
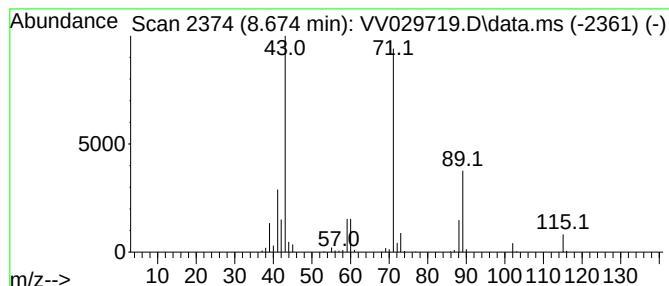
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.674	8.16 ug/L	207766	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	83
4		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW121922\
Data File : VV029719.D
Acq On : 19 Dec 2022 14:16
Operator : SY/MD
Sample : N6075-09 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSM5

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	12.9	ug/L	270314	1	5.609	1051340	50.0
Propanoic acid,...	7.182	2.7	ug/L	56628	1	5.609	1051340	50.0
Propanoic acid,...	7.918	2.9	ug/L	74596	2	8.844	1273700	50.0
Propanoic acid,...	8.188	4.9	ug/L	125784	2	8.844	1273700	50.0
Acetic acid, bu...	8.301	2.8	ug/L	71842	2	8.844	1273700	50.0
Isopropyl butyrate	8.674	8.2	ug/L	207766	2	8.844	1273700	50.0