

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
 Data File : VV029715.D
 Acq On : 19 Dec 2022 12:42
 Operator : SY/MD
 Sample : N6075-05 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGSL9

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: VV029715.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	75	82	99	rVB	222909	218835	14.57%	1.748%
2	1.561	155	162	179	rVB	178630	201293	13.40%	1.608%
3	2.105	320	331	343	rBV	355268	514235	34.23%	4.107%
4	2.503	445	455	467	rVB2	8708	14533	0.97%	0.116%
5	2.571	471	476	478	rBV2	347	316	0.02%	0.003%
6	2.603	483	486	488	rBV3	526	323	0.02%	0.003%
7	2.693	509	514	517	rVB	305	272	0.02%	0.002%
8	2.712	517	520	522	rBV2	138	90	0.01%	0.001%
9	2.725	522	524	528	rBV2	197	168	0.01%	0.001%
10	2.760	533	535	538	rVB	455	157	0.01%	0.001%
11	2.780	539	541	543	rVV	157	79	0.01%	0.001%
12	2.805	546	549	552	rVB2	223	139	0.01%	0.001%
13	2.896	574	577	584	rBV2	182	236	0.02%	0.002%
14	3.008	608	612	614	rBV2	228	175	0.01%	0.001%
15	3.079	632	634	638	rBV	135	66	0.00%	0.001%
16	3.130	647	650	653	rBV2	129	72	0.00%	0.001%
17	3.150	653	656	658	rBV2	106	72	0.00%	0.001%
18	3.175	658	664	667	rBV4	764	977	0.07%	0.008%
19	3.278	694	696	699	rBV2	137	84	0.01%	0.001%
20	3.336	710	714	719	rBV2	114	154	0.01%	0.001%
21	3.375	723	726	730	rBV2	123	77	0.01%	0.001%
22	3.394	730	732	734	rBV	103	60	0.00%	0.000%
23	3.407	734	736	743	rVB2	219	141	0.01%	0.001%
24	3.452	746	750	754	rBV	205	176	0.01%	0.001%
25	3.539	775	777	784	rBV	252	215	0.01%	0.002%
26	3.603	794	797	800	rBV2	145	122	0.01%	0.001%
27	3.622	800	803	806	rBV	277	192	0.01%	0.002%
28	3.703	825	828	830	rVB2	115	61	0.00%	0.000%
29	3.719	830	833	834	rBV	189	76	0.01%	0.001%
30	3.783	849	853	855	rBV2	131	115	0.01%	0.001%
31	3.825	863	866	870	rVB2	210	147	0.01%	0.001%
32	3.873	870	881	923	rBV2	99687	304270	20.25%	2.430%
33	4.336	1008	1025	1055	rBV	231118	575388	38.30%	4.595%
34	4.600	1105	1107	1109	rVB2	197	78	0.01%	0.001%
35	4.677	1128	1131	1132	rBV2	256	159	0.01%	0.001%
36	4.709	1139	1141	1145	rVB	191	131	0.01%	0.001%

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 Title : VOC Analysis

37	4.773	1158	1161	1164	rBV2	127	91	0.01%	0.001%
38	4.860	1185	1188	1193	rVV2	258	214	0.01%	0.002%
39	4.899	1197	1200	1206	rVB2	293	196	0.01%	0.002%
40	5.037	1222	1243	1283	rBV2	564104	1502308	100.00%	11.999%
41	5.281	1310	1319	1340	rBV2	10493	24891	1.66%	0.199%
42	5.468	1375	1377	1378	rBV	283	109	0.01%	0.001%
43	5.477	1378	1380	1381	rVV	253	93	0.01%	0.001%
44	5.609	1408	1421	1456	rBV	468380	971421	64.66%	7.758%
45	5.902	1502	1512	1519	rBV4	5595	10506	0.70%	0.084%
46	5.956	1527	1529	1535	rBV3	242	195	0.01%	0.002%
47	6.063	1548	1562	1599	rVV	322790	672302	44.75%	5.369%
48	6.304	1632	1637	1642	rVB2	450	479	0.03%	0.004%
49	6.346	1642	1650	1658	rBV2	4822	9769	0.65%	0.078%
50	6.458	1676	1685	1719	rBV	123232	240041	15.98%	1.917%
51	6.812	1790	1795	1796	rBV2	343	287	0.02%	0.002%
52	6.837	1800	1803	1805	rBV	171	120	0.01%	0.001%
53	6.918	1826	1828	1831	rVB2	243	110	0.01%	0.001%
54	6.979	1834	1847	1879	rBV	164526	307951	20.50%	2.460%
55	7.182	1899	1910	1921	rBV	32066	55682	3.71%	0.445%
56	7.307	1937	1949	1979	rBV	707906	1255875	83.60%	10.030%
57	7.612	2034	2044	2063	rBV2	144512	254991	16.97%	2.037%
58	7.821	2105	2109	2110	rBV2	572	371	0.02%	0.003%
59	7.918	2127	2139	2159	rBV	39781	70124	4.67%	0.560%
60	8.082	2181	2190	2215	rBV	348276	632099	42.08%	5.048%
61	8.185	2216	2222	2239	rVB	65147	106381	7.08%	0.850%
62	8.297	2249	2257	2276	rVB	31530	54887	3.65%	0.438%
63	8.545	2332	2334	2341	rVB4	444	352	0.02%	0.003%
64	8.574	2341	2343	2345	rBV2	464	237	0.02%	0.002%
65	8.673	2364	2374	2400	rBV	121648	194897	12.97%	1.557%
66	8.844	2414	2427	2450	rBV	708187	1163923	77.48%	9.296%
67	9.117	2505	2512	2515	rBV5	1279	1434	0.10%	0.011%
68	9.178	2528	2531	2535	rBV2	290	285	0.02%	0.002%
69	9.239	2546	2550	2554	rBV2	317	355	0.02%	0.003%
70	9.294	2565	2567	2573	rVB2	283	208	0.01%	0.002%
71	9.384	2587	2595	2603	rBV5	1512	2437	0.16%	0.019%
72	9.542	2636	2644	2658	rVB4	8656	14441	0.96%	0.115%
73	9.625	2669	2670	2671	rBV4	205	56	0.00%	0.000%
74	9.657	2674	2680	2685	rVB2	321	375	0.02%	0.003%
75	9.741	2704	2706	2710	rBV2	182	88	0.01%	0.001%
76	9.911	2757	2759	2762	rBV	302	133	0.01%	0.001%

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77	9.963	2771	2775	2778	rBV	220	179	0.01%	0.001%
78	10.069	2805	2808	2810	rBV2	188	84	0.01%	0.001%
79	10.162	2827	2837	2840	rBV2	17877	24174	1.61%	0.193%
80	10.204	2841	2850	2871	rVB	457325	724336	48.21%	5.785%
81	10.333	2888	2890	2891	rBV	122	56	0.00%	0.000%
82	10.371	2898	2902	2912	rVB2	1341	1874	0.12%	0.015%
83	10.529	2945	2951	2953	rBV4	793	745	0.05%	0.006%
84	10.567	2956	2963	2979	rVB2	8977	14518	0.97%	0.116%
85	10.664	2989	2993	2996	rBV2	251	220	0.01%	0.002%
86	10.754	3017	3021	3024	rBV2	233	220	0.01%	0.002%
87	10.995	3093	3096	3099	rBV2	261	135	0.01%	0.001%
88	11.011	3099	3101	3104	rBV	196	78	0.01%	0.001%
89	11.075	3119	3121	3123	rVB	335	129	0.01%	0.001%
90	11.168	3147	3150	3157	rBV3	570	561	0.04%	0.004%
91	11.236	3159	3171	3193	rBV	761221	1190600	79.25%	9.509%
92	11.541	3265	3266	3268	rVB	257	86	0.01%	0.001%
93	11.612	3276	3288	3313	rBV	751920	1168515	77.78%	9.333%
94	11.905	3375	3379	3383	rBV3	410	387	0.03%	0.003%
95	12.001	3405	3409	3418	rVB5	1049	1446	0.10%	0.012%
96	12.368	3520	3523	3529	rBV2	396	469	0.03%	0.004%
97	12.397	3529	3532	3533	rBV2	811	425	0.03%	0.003%
98	12.869	3673	3679	3688	rVB3	3003	4083	0.27%	0.033%
99	12.966	3706	3709	3712	rBV2	575	473	0.03%	0.004%
100	13.258	3792	3800	3808	rBV6	1964	2602	0.17%	0.021%

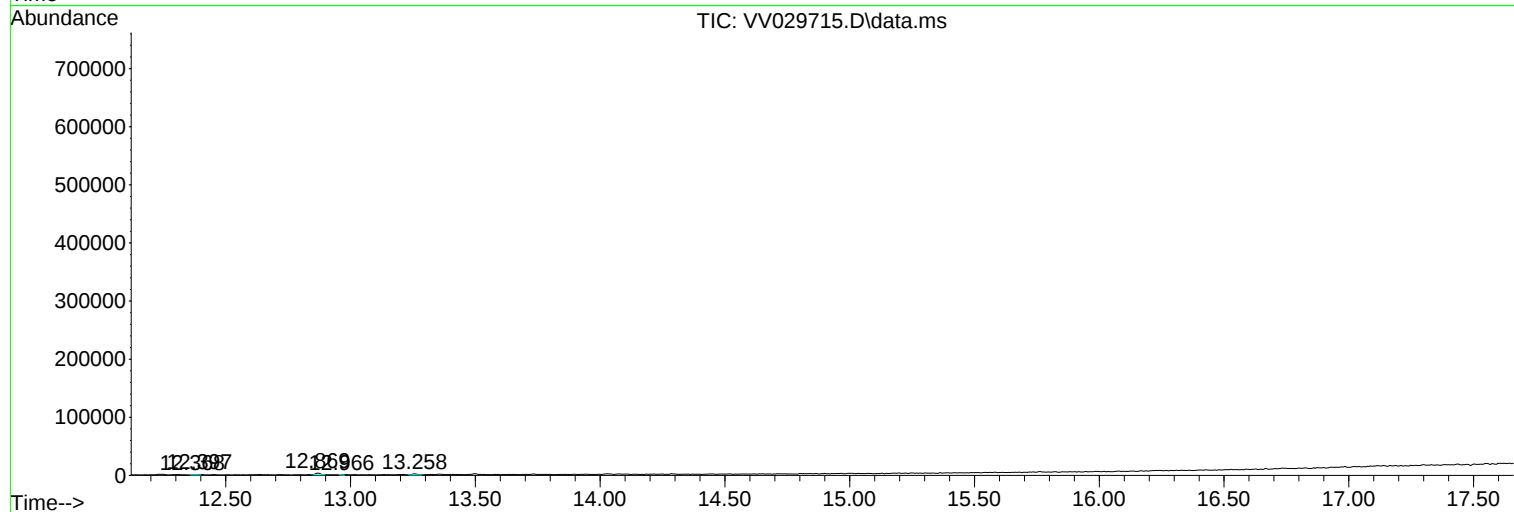
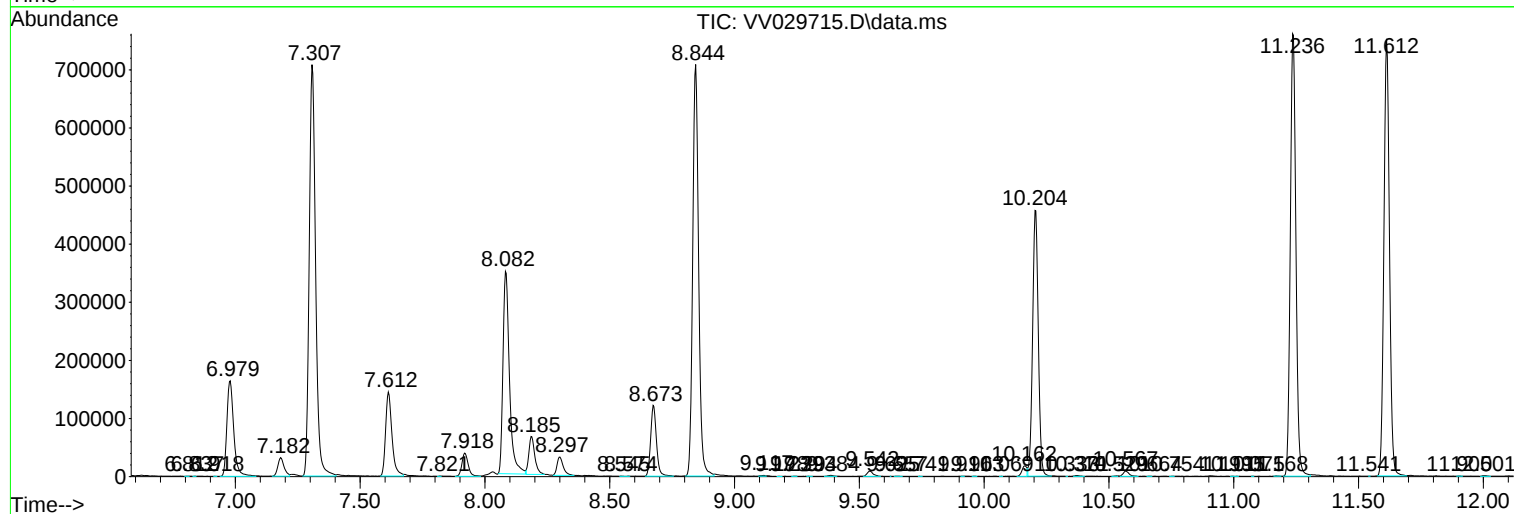
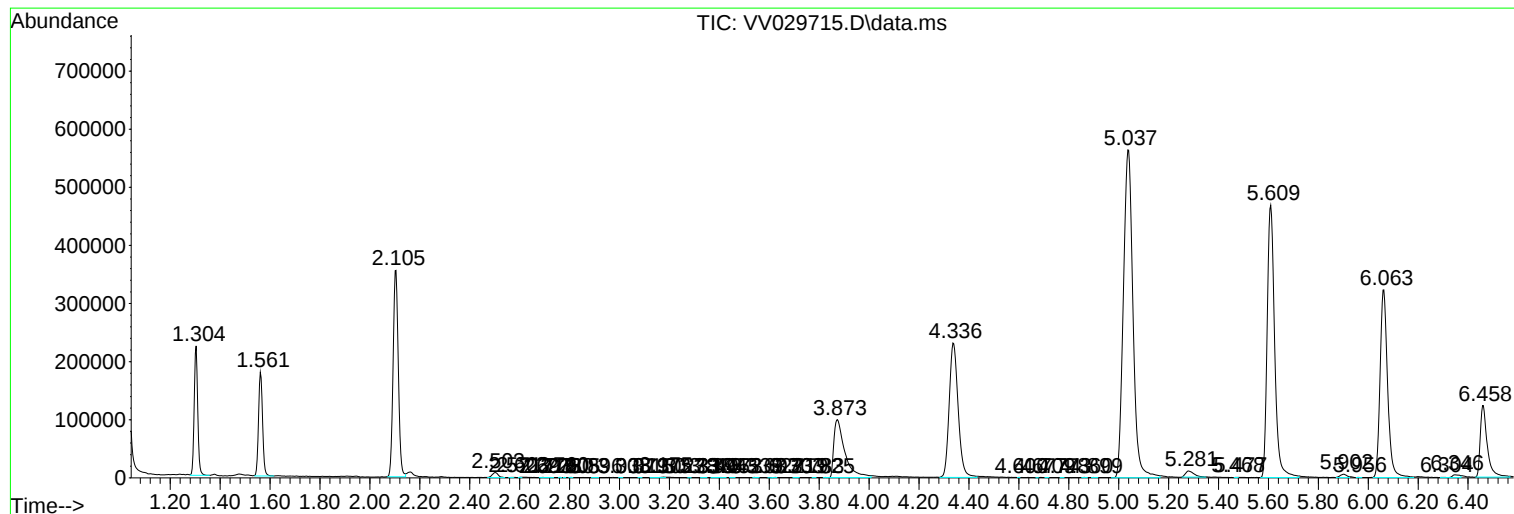
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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



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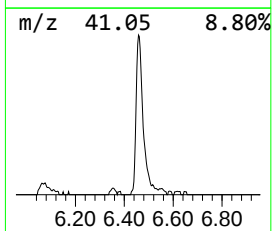
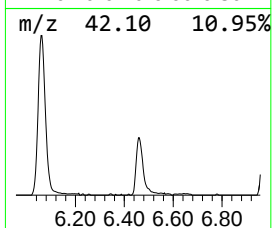
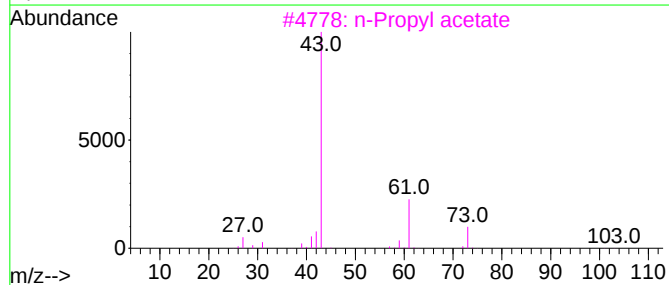
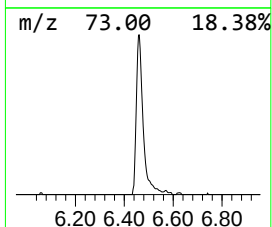
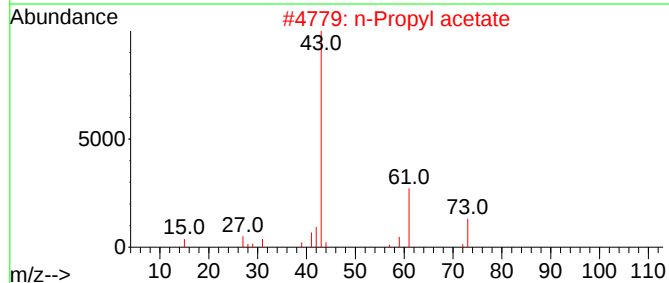
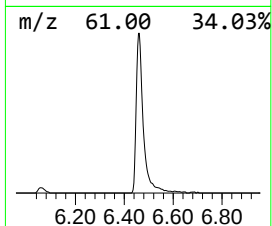
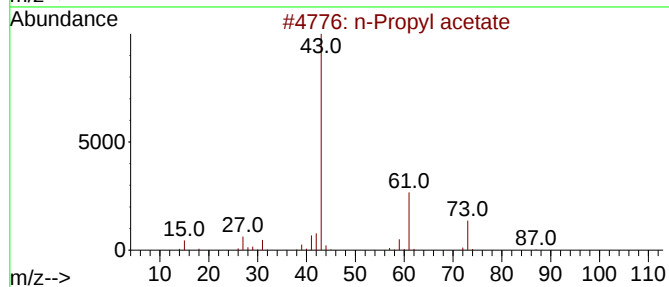
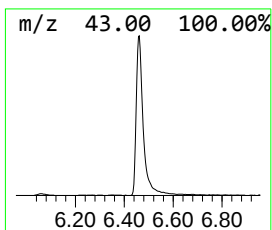
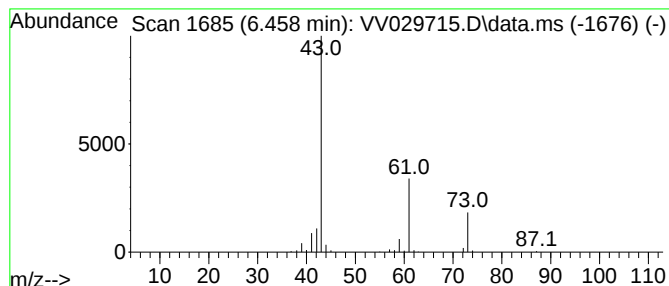
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.458	12.36 ug/L	240041	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	78	
4	n-Propyl acetate	102	C5H10O2	000109-60-4	72	
5	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	33	



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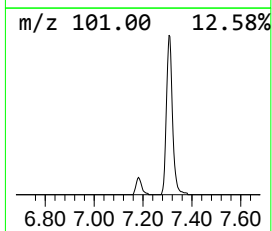
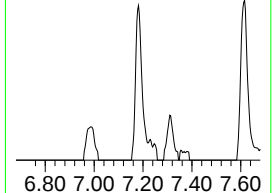
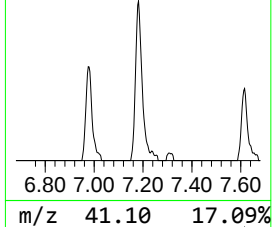
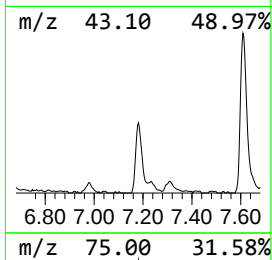
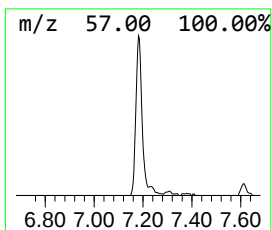
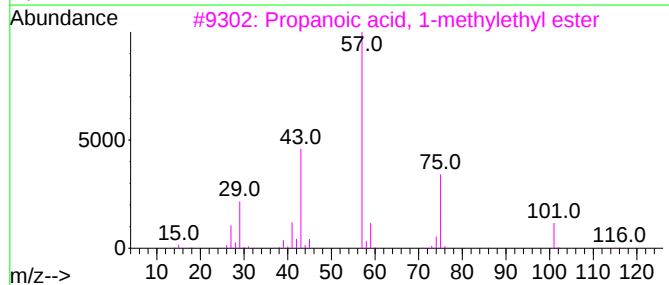
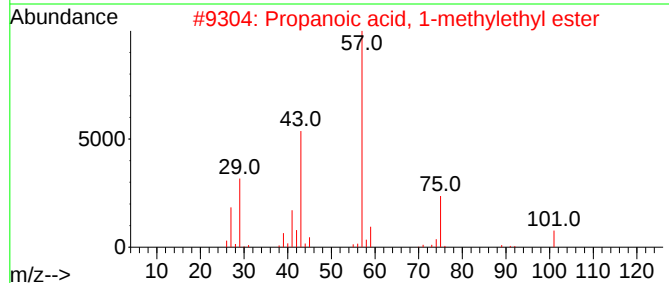
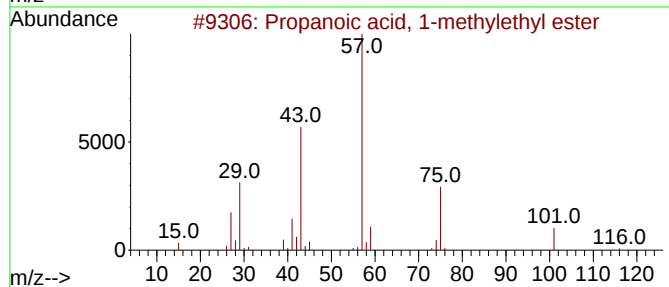
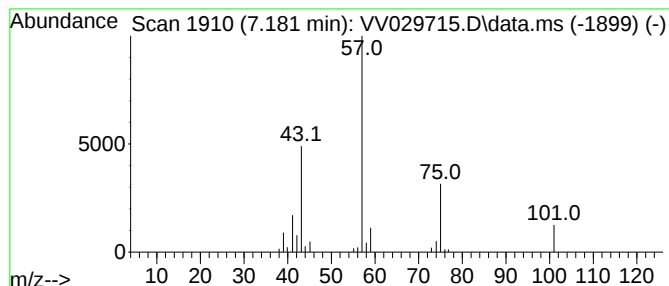
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.181	2.87 ug/L	55682	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	53



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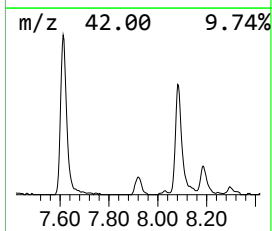
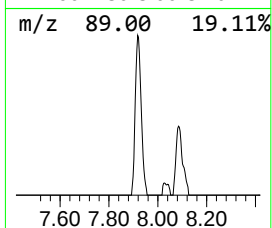
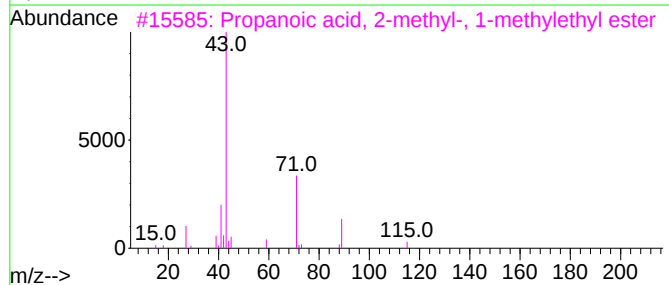
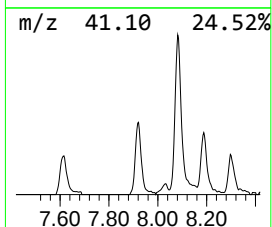
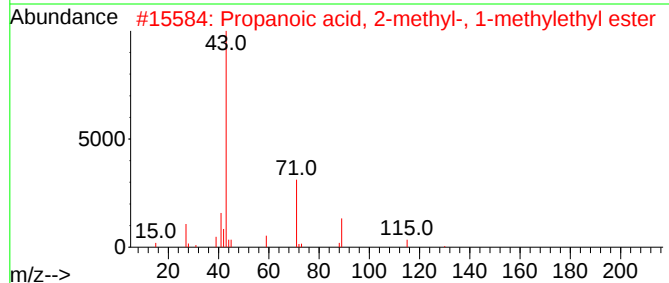
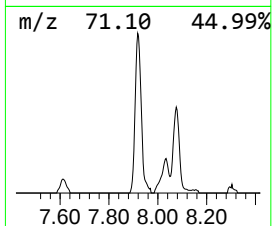
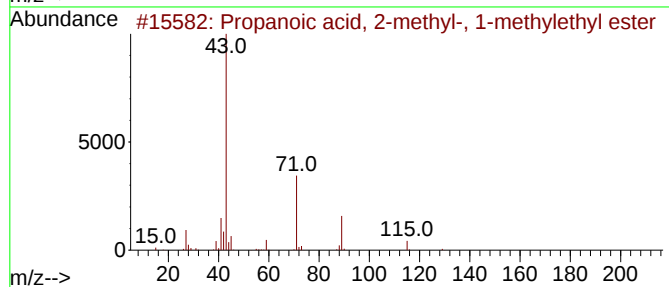
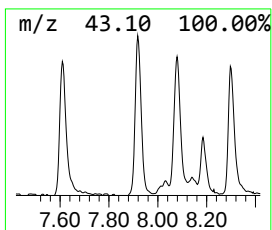
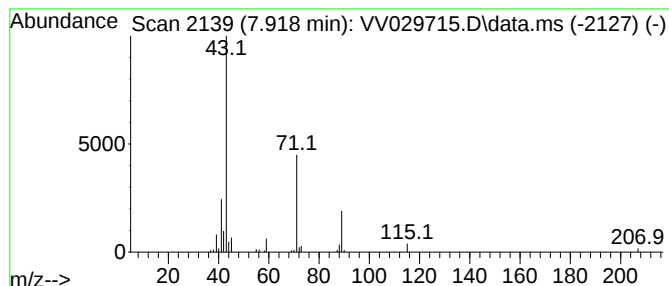
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.918	3.01 ug/L	70124	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	83
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 : VV029715.D
Acq On : 19 Dec 2022 12:42
Operator : SY/MD
Sample : N6075-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGS9

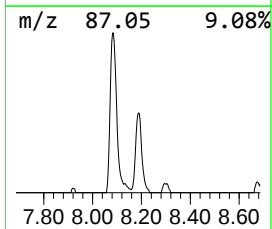
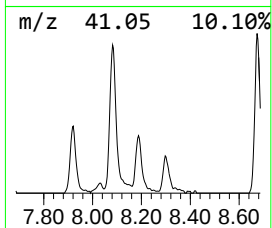
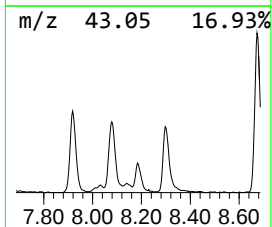
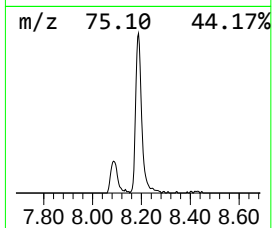
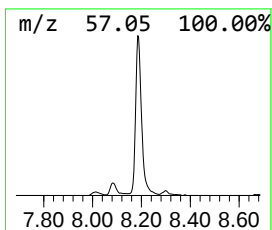
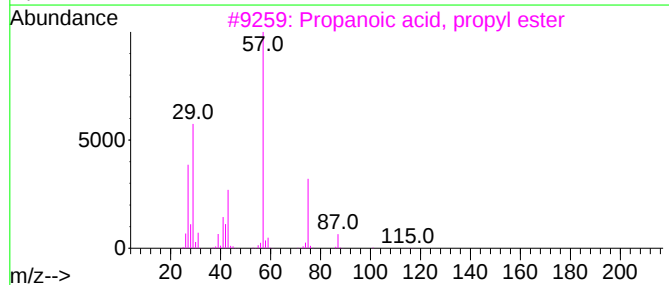
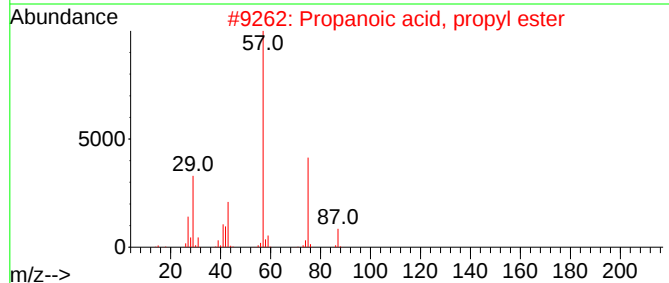
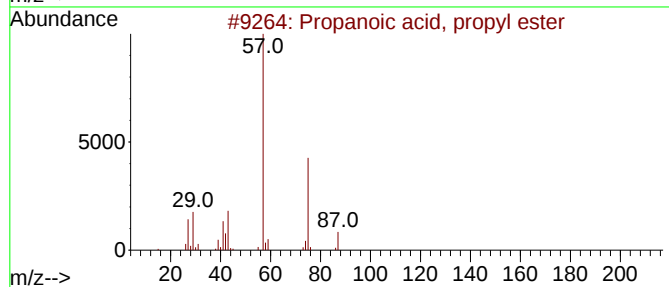
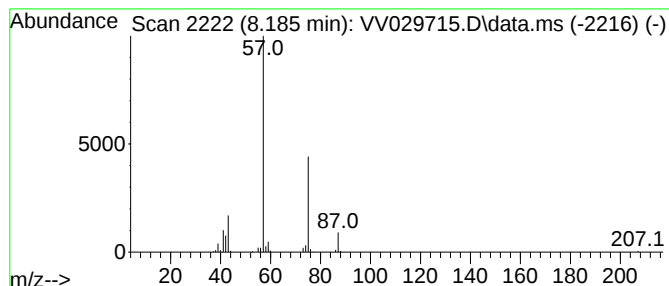
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Quant Title : VOC Analysis

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.
8.185	4.57 ug/L	106381	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	78
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029715.D
Acq On : 19 Dec 2022 12:42
Operator : SY/MD
Sample : N6075-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSL9

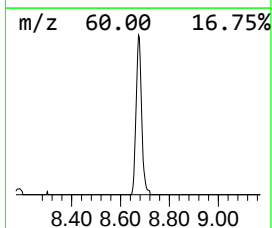
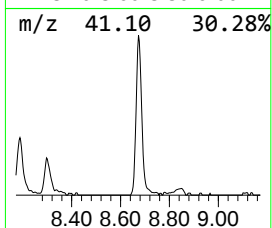
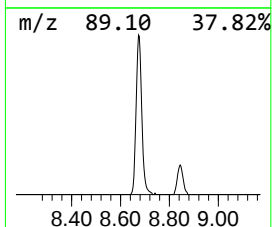
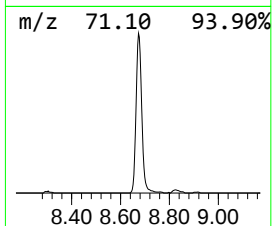
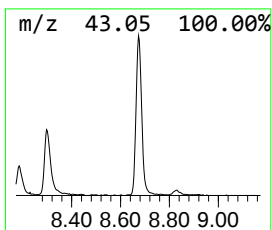
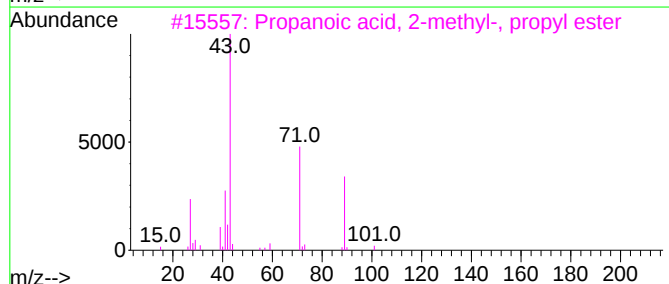
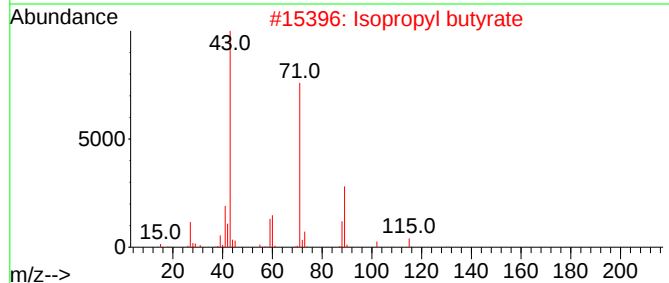
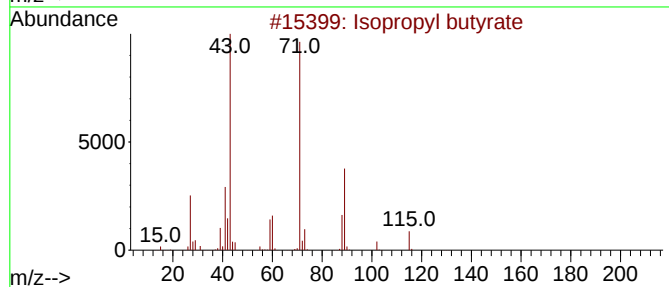
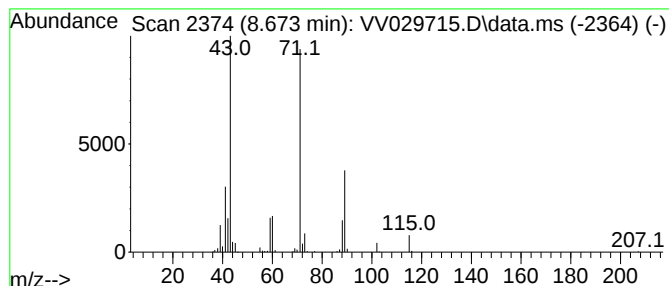
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120722WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.673	8.37 ug/L	194897	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			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121922\
Data File : VV029715.D
Acq On : 19 Dec 2022 12:42
Operator : SY/MD
Sample : N6075-05 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGSL9

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.458	12.4	ug/L	240041	1	5.609	971421	50.0
Propanoic acid,...	7.181	2.9	ug/L	55682	1	5.609	971421	50.0
Propanoic acid,...	7.918	3.0	ug/L	70124	2	8.844	1163920	50.0
Propanoic acid,...	8.185	4.6	ug/L	106381	2	8.844	1163920	50.0
Isopropyl butyrate	8.673	8.4	ug/L	194897	2	8.844	1163920	50.0