

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050124\
 Data File : VV035502.D
 Acq On : 01 May 2024 17:28
 Operator : SY/MD
 Sample : PB160591TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB591

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\SFAMVLM050124WMA.M

Title : VOC Analysis

Signal : TIC: VV035502.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	67	74	92	rVB	271215	294541	15.24%	1.850%
2	1.529	145	152	180	rVB	244946	300549	15.55%	1.887%
3	2.056	306	316	330	rBV	460718	660453	34.16%	4.147%
4	2.281	383	386	390	rBV4	888	763	0.04%	0.005%
5	2.445	429	437	450	rVB2	6850	11274	0.58%	0.071%
6	2.558	463	472	481	rBV3	898	1659	0.09%	0.010%
7	2.696	512	515	517	rBV3	463	275	0.01%	0.002%
8	2.841	556	560	563	rBV3	290	237	0.01%	0.001%
9	3.040	618	622	626	rBV2	237	213	0.01%	0.001%
10	3.124	641	648	653	rBV3	986	1470	0.08%	0.009%
11	3.214	673	676	682	rVB2	323	306	0.02%	0.002%
12	3.246	682	686	689	rBV2	341	283	0.01%	0.002%
13	3.272	689	694	696	rBV	317	231	0.01%	0.001%
14	3.304	700	704	708	rBV2	204	233	0.01%	0.001%
15	3.449	745	749	753	rBV	329	240	0.01%	0.002%
16	3.789	846	855	902	rBV	138248	421594	21.81%	2.647%
17	4.246	980	997	1035	rBV	306291	790183	40.88%	4.962%
18	4.703	1136	1139	1143	rVB2	387	276	0.01%	0.002%
19	4.767	1156	1159	1161	rBV2	350	224	0.01%	0.001%
20	4.860	1182	1188	1190	rBV2	476	394	0.02%	0.002%
21	4.953	1201	1217	1260	rBV2	739022	1933134	100.00%	12.139%
22	5.217	1290	1299	1318	rBV2	8877	23716	1.23%	0.149%
23	5.413	1357	1360	1364	rBV2	619	563	0.03%	0.004%
24	5.532	1386	1397	1433	rBV	561656	1180503	61.07%	7.413%
25	5.831	1482	1490	1502	rBV6	4725	10821	0.56%	0.068%
26	5.985	1526	1538	1569	rBV	422243	868986	44.95%	5.457%
27	6.313	1625	1640	1643	rBV2	4165	8538	0.44%	0.054%
28	6.394	1657	1665	1712	rBV	145960	299078	15.47%	1.878%
29	6.873	1812	1814	1816	rBV2	474	239	0.01%	0.002%
30	6.911	1816	1826	1850	rBV	221365	416838	21.56%	2.618%
31	7.120	1882	1891	1909	rBV	34762	64121	3.32%	0.403%
32	7.239	1917	1928	1973	rBV	860382	1540379	79.68%	9.673%
33	7.551	2016	2025	2053	rBV2	190486	361305	18.69%	2.269%
34	7.863	2110	2122	2142	rBV	46132	85898	4.44%	0.539%
35	7.976	2148	2157	2162	rBV4	10709	16467	0.85%	0.103%
36	8.024	2162	2172	2197	rVV	517339	948896	49.09%	5.959%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050124\
 Data File : VV035502.D
 Acq On : 01 May 2024 17:28
 Operator : SY/MD
 Sample : PB160591TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB591

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\SFAMVLM050124WMA.M
 Title : VOC Analysis

37	8.130	2198	2205	2231	rVV	82880	162966	8.43%	1.023%
38	8.246	2234	2241	2271	rVB2	40291	82557	4.27%	0.518%
39	8.619	2347	2357	2378	rVV	135329	222713	11.52%	1.399%
40	8.783	2397	2408	2444	rBV	916865	1494533	77.31%	9.385%
41	9.246	2550	2552	2556	rVB2	457	300	0.02%	0.002%
42	9.275	2556	2561	2564	rBV5	671	608	0.03%	0.004%
43	9.349	2577	2584	2585	rBV3	634	560	0.03%	0.004%
44	9.432	2608	2610	2614	rVB3	559	336	0.02%	0.002%
45	9.468	2618	2621	2623	rBV2	556	435	0.02%	0.003%
46	9.500	2623	2631	2644	rBV3	7035	12806	0.66%	0.080%
47	9.657	2678	2680	2682	rBV2	375	246	0.01%	0.002%
48	9.873	2744	2747	2753	rBV3	794	800	0.04%	0.005%
49	9.911	2757	2759	2763	rVB3	410	270	0.01%	0.002%
50	9.937	2763	2767	2772	rBV	285	276	0.01%	0.002%
51	9.982	2776	2781	2786	rBV3	533	811	0.04%	0.005%
52	10.017	2789	2792	2795	rVB4	427	312	0.02%	0.002%
53	10.037	2795	2798	2804	rBV3	459	306	0.02%	0.002%
54	10.149	2821	2833	2862	rBV	646445	1023273	52.93%	6.426%
55	10.320	2881	2886	2899	rVB3	3750	6140	0.32%	0.039%
56	10.374	2901	2903	2906	rVB2	408	250	0.01%	0.002%
57	10.487	2934	2938	2939	rBV2	542	429	0.02%	0.003%
58	10.509	2944	2945	2951	rVB3	417	308	0.02%	0.002%
59	10.561	2958	2961	2965	rBV3	507	341	0.02%	0.002%
60	10.644	2982	2987	2989	rBV2	340	324	0.02%	0.002%
61	10.661	2989	2992	2997	rVB3	358	227	0.01%	0.001%
62	10.808	3036	3038	3041	rBV2	423	234	0.01%	0.001%
63	10.863	3051	3055	3059	rVB2	444	392	0.02%	0.002%
64	11.124	3133	3136	3140	rBV2	602	600	0.03%	0.004%
65	11.185	3144	3155	3182	rBV	819948	1291307	66.80%	8.109%
66	11.455	3236	3239	3241	rBV	471	340	0.02%	0.002%
67	11.490	3248	3250	3254	rVB2	453	331	0.02%	0.002%
68	11.509	3254	3256	3258	rVB2	541	253	0.01%	0.002%
69	11.558	3258	3271	3295	rBV	860570	1361819	70.45%	8.552%
70	11.837	3355	3358	3365	rBV2	447	540	0.03%	0.003%
71	11.869	3365	3368	3375	rVV6	488	554	0.03%	0.003%
72	11.934	3385	3388	3391	rVB2	758	427	0.02%	0.003%
73	11.995	3404	3407	3411	rBV3	310	266	0.01%	0.002%
74	12.133	3447	3450	3453	rBV4	305	245	0.01%	0.002%
75	12.194	3464	3469	3476	rVV6	950	1383	0.07%	0.009%
76	12.233	3478	3481	3485	rVB3	385	276	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050124\
Data File : VV035502.D
Acq On : 01 May 2024 17:28
Operator : SY/MD
Sample : PB160591TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB591

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050124WMA.M

Title : VOC Analysis

77	12.365	3519	3522	3527	rBV2	287	257	0.01%	0.002%
78	12.435	3542	3544	3548	rVB2	348	279	0.01%	0.002%
79	12.461	3548	3552	3556	rVB3	513	491	0.03%	0.003%
80	12.551	3577	3580	3584	rVB2	311	241	0.01%	0.002%
81	12.593	3589	3593	3602	rBV5	900	961	0.05%	0.006%
82	12.632	3602	3605	3608	rBV2	407	267	0.01%	0.002%
83	12.651	3608	3611	3614	rBV3	441	319	0.02%	0.002%
84	12.715	3628	3631	3637	rVB4	801	711	0.04%	0.004%
85	12.744	3637	3640	3643	rBV3	661	532	0.03%	0.003%
86	12.805	3656	3659	3663	rVV3	496	398	0.02%	0.002%
87	12.844	3668	3671	3677	rBV3	413	328	0.02%	0.002%
88	12.873	3677	3680	3683	rBV3	572	372	0.02%	0.002%
89	12.931	3697	3698	3702	rBV2	340	279	0.01%	0.002%
90	12.998	3715	3719	3720	rBV2	381	261	0.01%	0.002%
91	13.072	3738	3742	3745	rVV	389	319	0.02%	0.002%
92	13.111	3751	3754	3756	rBV2	464	321	0.02%	0.002%
93	13.201	3779	3782	3783	rBV	371	233	0.01%	0.001%
94	13.451	3856	3860	3861	rBV3	454	363	0.02%	0.002%
95	13.844	3977	3982	3983	rBV2	389	259	0.01%	0.002%
96	13.873	3989	3991	3994	rVB	433	217	0.01%	0.001%
97	14.242	4103	4106	4107	rBV	509	299	0.02%	0.002%
98	14.538	4196	4198	4200	rBV3	483	238	0.01%	0.001%
99	14.686	4241	4244	4247	rBV3	517	398	0.02%	0.002%
100	15.316	4438	4440	4442	rBV2	801	410	0.02%	0.003%

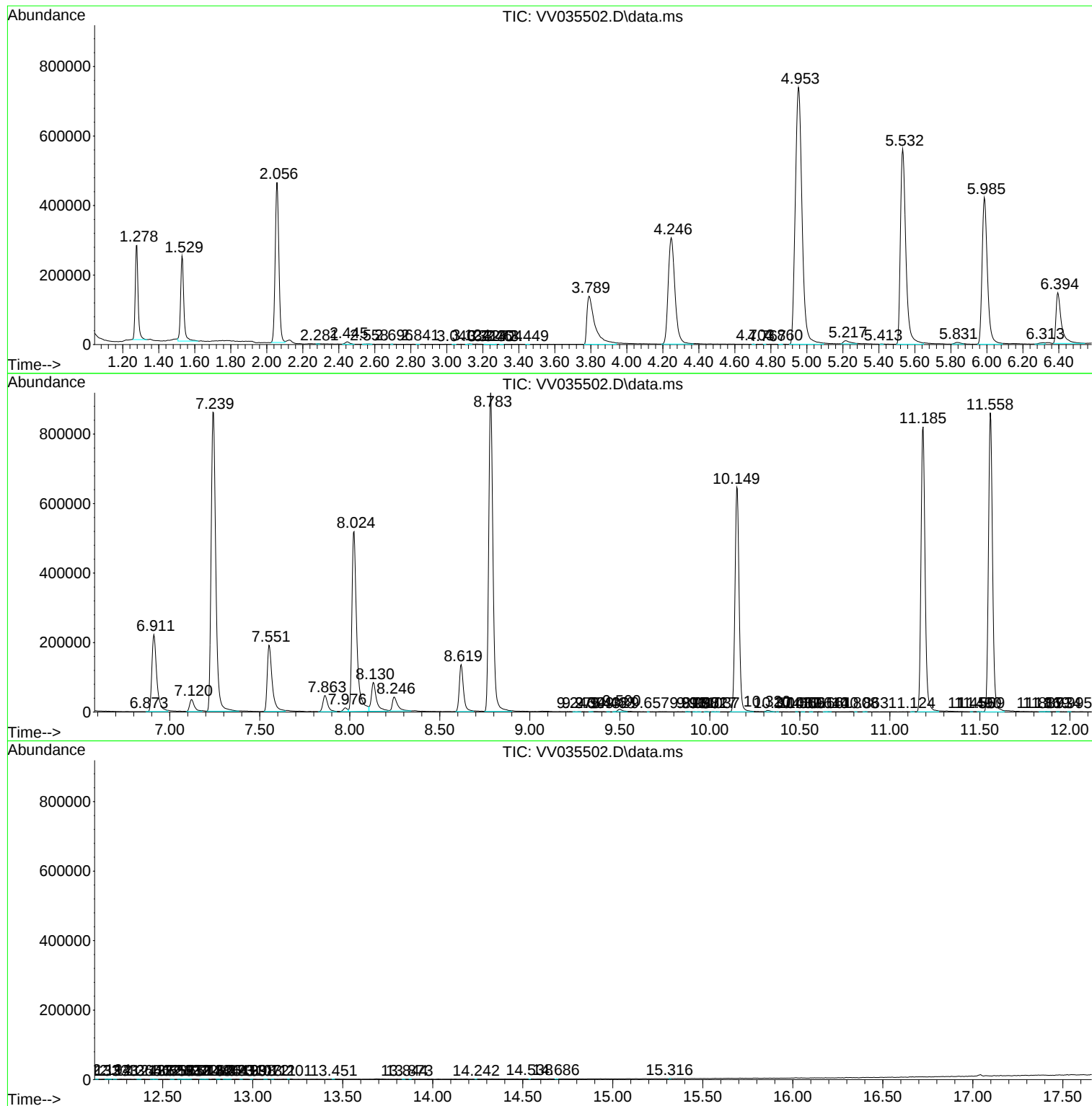
Sum of corrected areas: 15924727

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050124\
Data File : VV035502.D
Acq On : 01 May 2024 17:28
Operator : SY/MD
Sample : PB160591TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB591

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050124WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050124\
Data File : VV035502.D
Acq On : 01 May 2024 17:28
Operator : SY/MD
Sample : PB160591TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB591

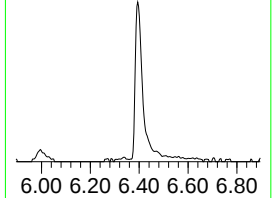
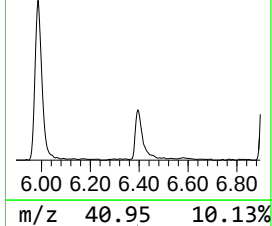
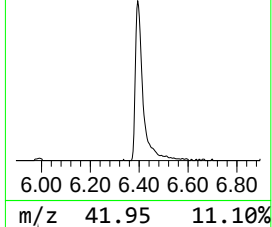
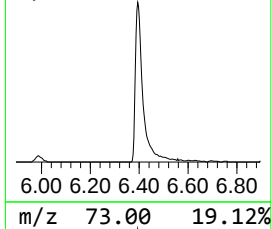
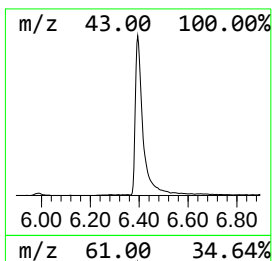
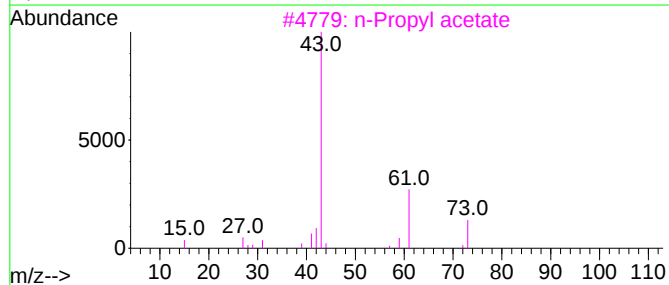
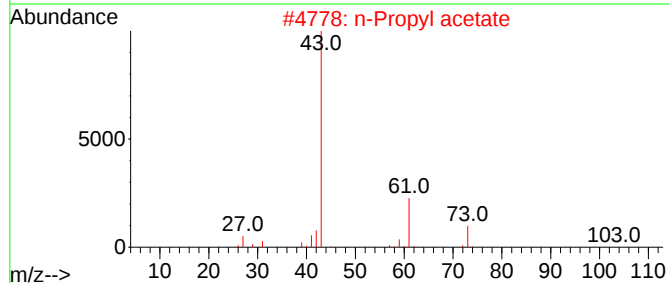
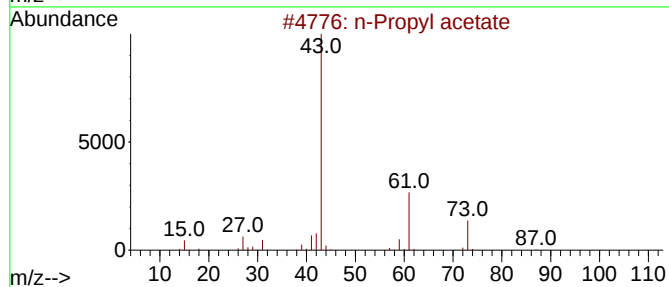
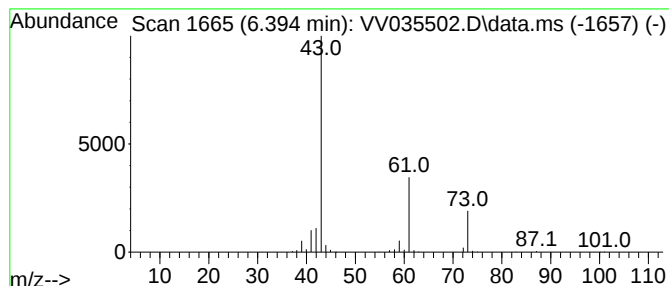
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050124WMA.M
Quant Title : VOC Analysis

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.
6.394	12.67 ug/L	299078	1,4-Difluorobenzene	5.532

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	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050124\
Data File : VV035502.D
Acq On : 01 May 2024 17:28
Operator : SY/MD
Sample : PB160591TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB591

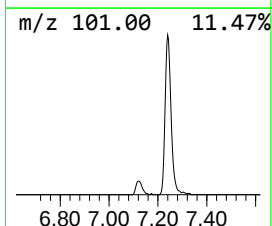
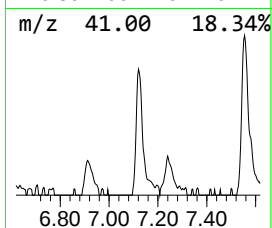
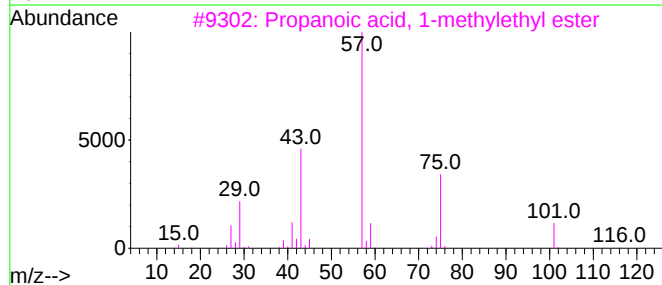
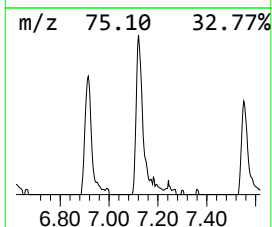
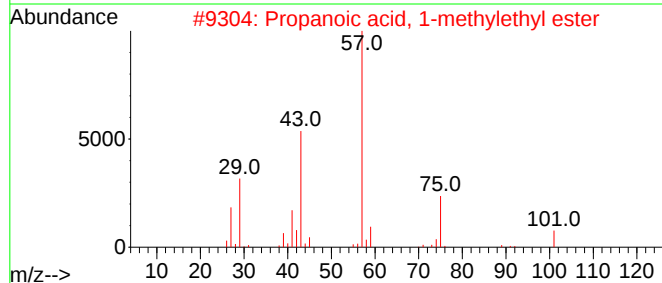
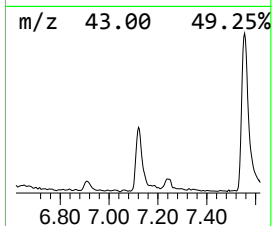
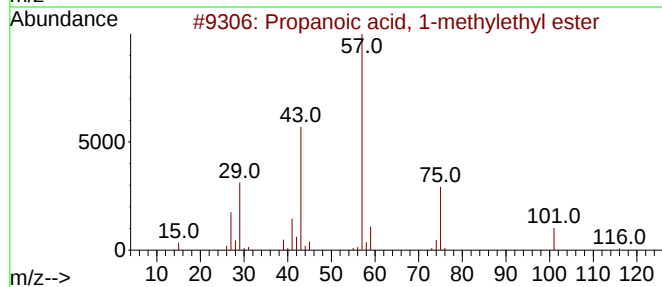
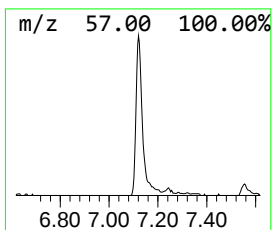
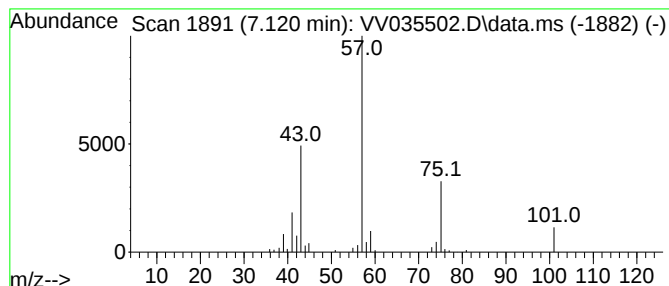
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050124WMA.M
Quant Title : VOC Analysis

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.
7.120	2.72 ug/L	64121	1,4-Difluorobenzene	5.532

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, propyl ester	116	C6H12O2	000106-36-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050124\
Data File : VV035502.D
Acq On : 01 May 2024 17:28
Operator : SY/MD
Sample : PB160591TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB591

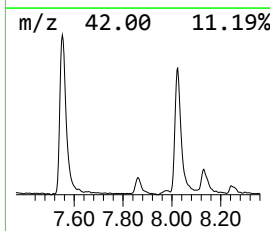
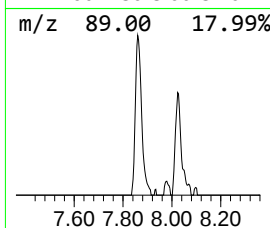
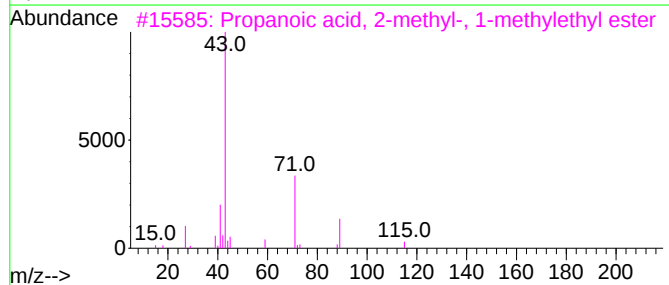
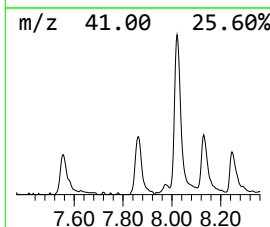
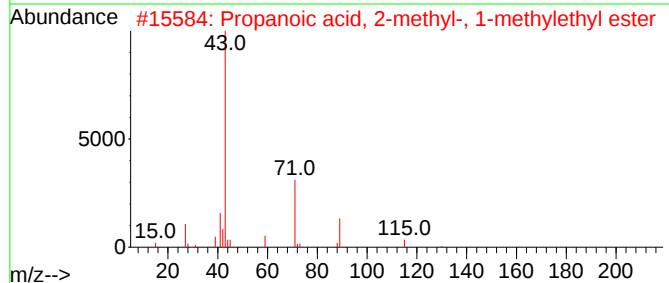
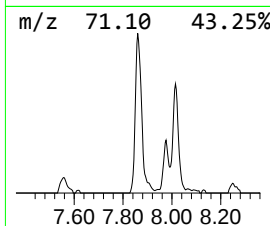
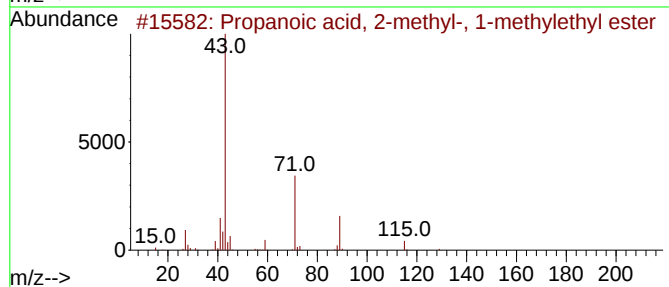
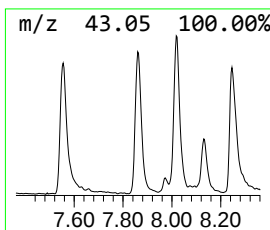
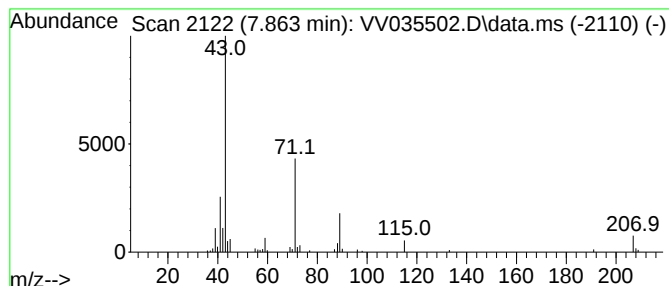
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050124WMA.M
Quant Title : VOC Analysis

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.
7.863	2.87 ug/L	85898	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050124\
Data File : VV035502.D
Acq On : 01 May 2024 17:28
Operator : SY/MD
Sample : PB160591TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB591

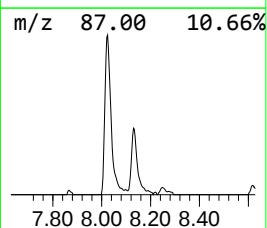
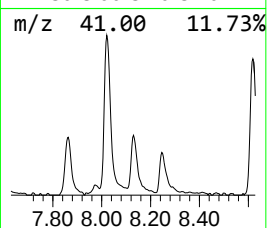
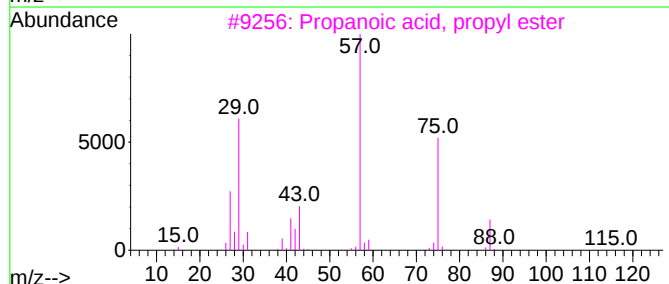
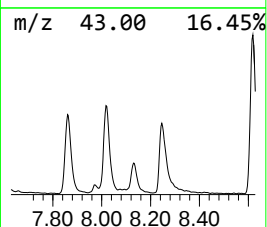
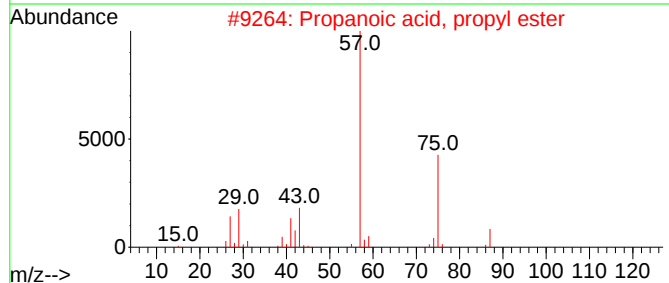
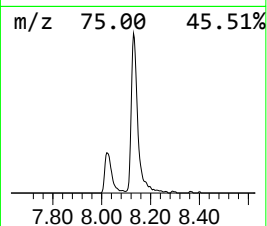
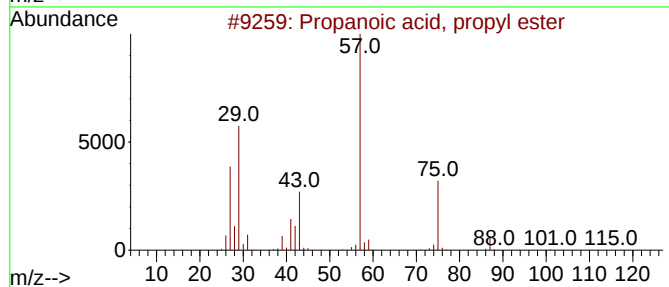
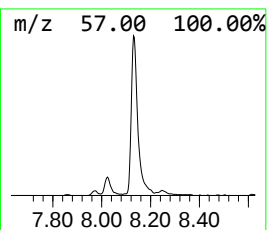
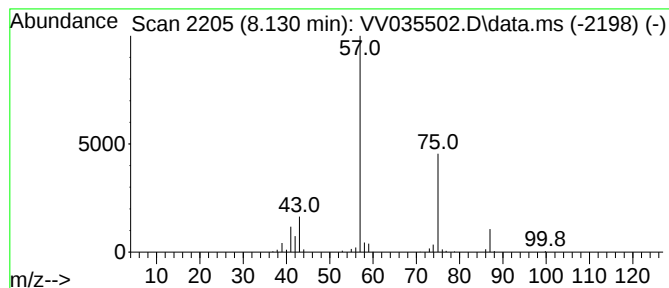
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050124WMA.M
Quant Title : VOC Analysis

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.
8.130	5.45 ug/L	162966	Chlorobenzene-d5	8.783

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, butyl ester	130	C7H14O2	000590-01-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050124\
Data File : VV035502.D
Acq On : 01 May 2024 17:28
Operator : SY/MD
Sample : PB160591TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB591

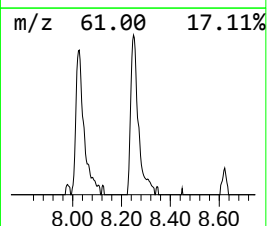
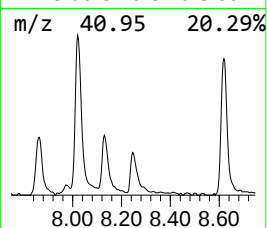
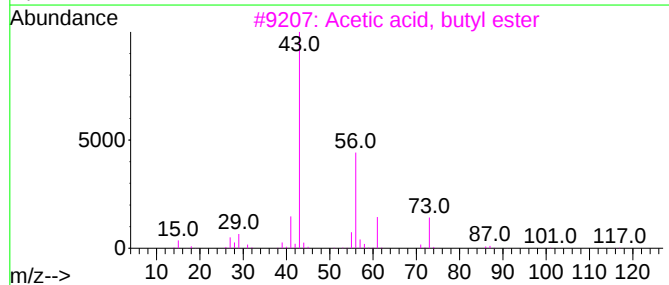
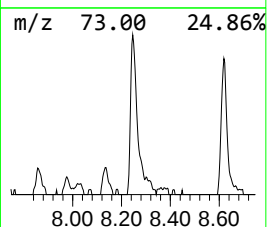
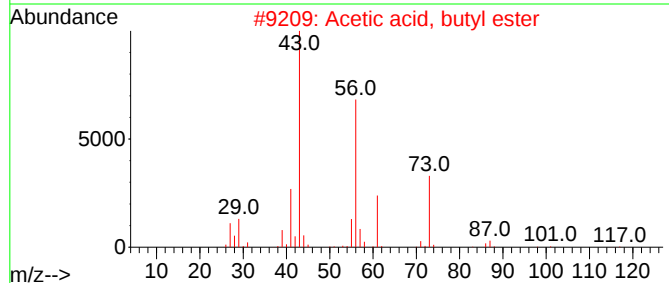
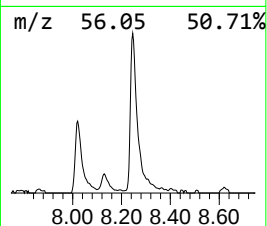
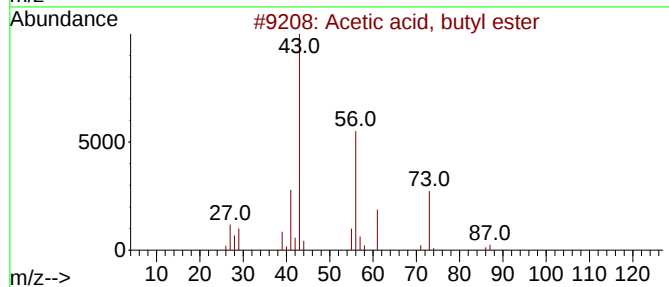
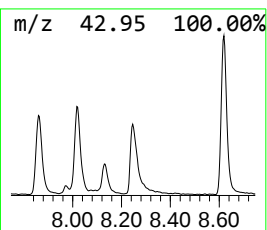
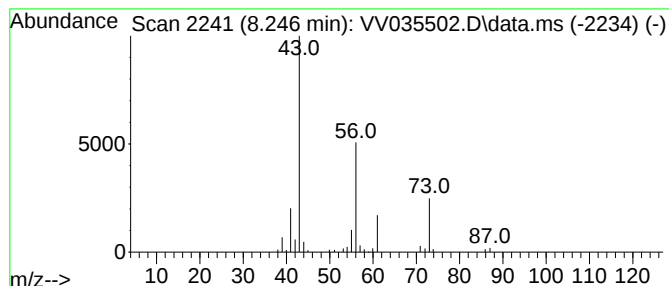
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050124WMA.M
Quant Title : VOC Analysis

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.
8.246	2.76 ug/L	82557	Chlorobenzene-d5	8.783

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	50		
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	33		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050124\
Data File : VV035502.D
Acq On : 01 May 2024 17:28
Operator : SY/MD
Sample : PB160591TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB591

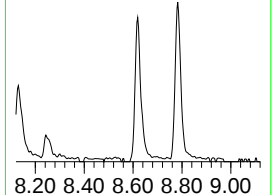
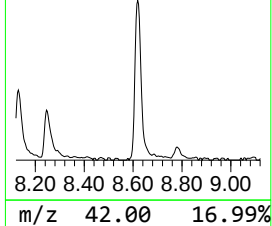
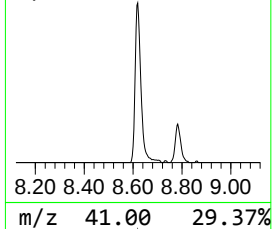
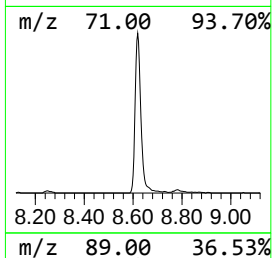
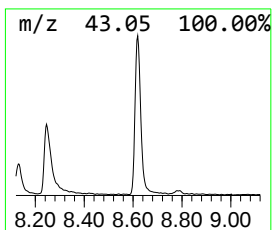
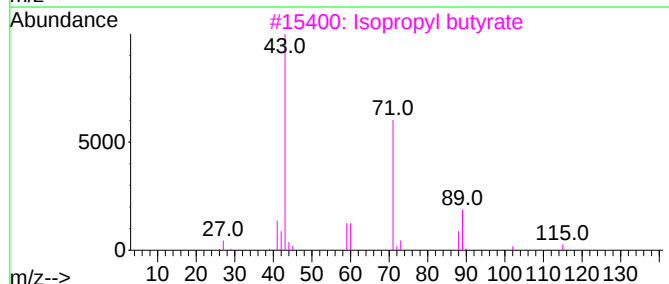
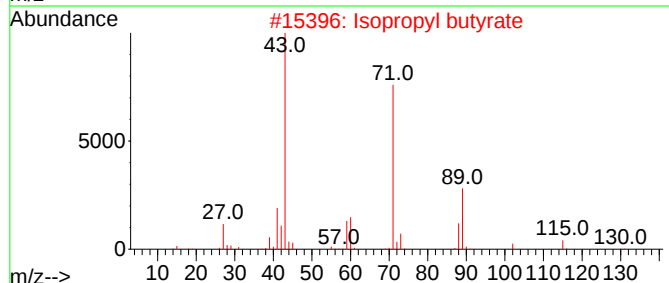
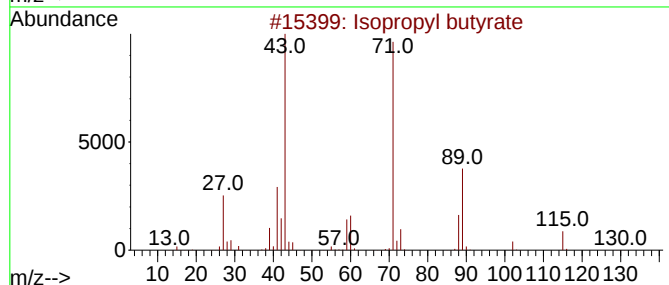
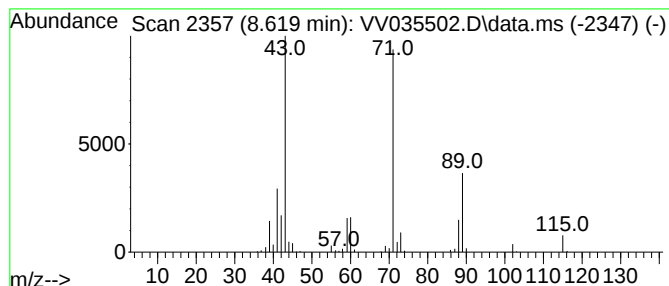
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050124WMA.M
Quant Title : VOC Analysis

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.
8.619	7.45 ug/L	222713	Chlorobenzene-d5	8.783

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			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050124\
Data File : VV035502.D
Acq On : 01 May 2024 17:28
Operator : SY/MD
Sample : PB160591TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB591

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050124WMA.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	6.394	12.7	ug/L	299078	1	5.532	1180500	50.0
Propanoic acid,...	7.120	2.7	ug/L	64121	1	5.532	1180500	50.0
Propanoic acid,...	7.863	2.9	ug/L	85898	2	8.783	1494530	50.0
Propanoic acid,...	8.130	5.5	ug/L	162966	2	8.783	1494530	50.0
Acetic acid, bu...	8.246	2.8	ug/L	82557	2	8.783	1494530	50.0
Isopropyl butyrate	8.619	7.5	ug/L	222713	2	8.783	1494530	50.0