

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
 Data File : VN068504.D
 Acq On : 16 Sep 2021 19:10
 Operator : JC/MD
 Sample : M3759-17 10X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31185

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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_N\methods\82N090721W.M

Title : SW846 8260

Signal : TIC: VN068504.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.236	78	92	112	rBV3	107070	192673	3.80%	0.899%
2	2.588	208	223	252	rBV	923425	1661076	32.76%	7.748%
3	4.149	783	805	833	rBV	61658	181503	3.58%	0.847%
4	4.291	839	858	885	rBV	55579	159754	3.15%	0.745%
5	4.575	942	964	996	rBV2	33880	111634	2.20%	0.521%
6	7.155	1909	1926	1956	rVB2	72855	204395	4.03%	0.953%
7	8.024	2228	2250	2261	rBV	327296	783786	15.46%	3.656%
8	8.088	2262	2274	2304	rVB	636167	1457387	28.74%	6.798%
9	8.440	2384	2405	2433	rBV	310144	731226	14.42%	3.411%
10	8.973	2580	2604	2652	rBV3	2351158	5070952	100.00%	23.654%
11	9.215	2676	2694	2741	rVB	1282053	2602772	51.33%	12.141%
12	10.443	3130	3152	3170	rBV	1208433	2297775	45.31%	10.718%
13	10.690	3226	3244	3280	rBV2	279412	589620	11.63%	2.750%
14	10.832	3280	3297	3316	rVB2	28335	54118	1.07%	0.252%
15	11.143	3401	3413	3424	rBV	66109	119156	2.35%	0.556%
16	11.747	3610	3638	3667	rBV	1084265	2023696	39.91%	9.440%
17	12.733	3990	4006	4036	rVB	842819	1485950	29.30%	6.931%
18	13.678	4342	4358	4382	rVB	986807	1710728	33.74%	7.980%

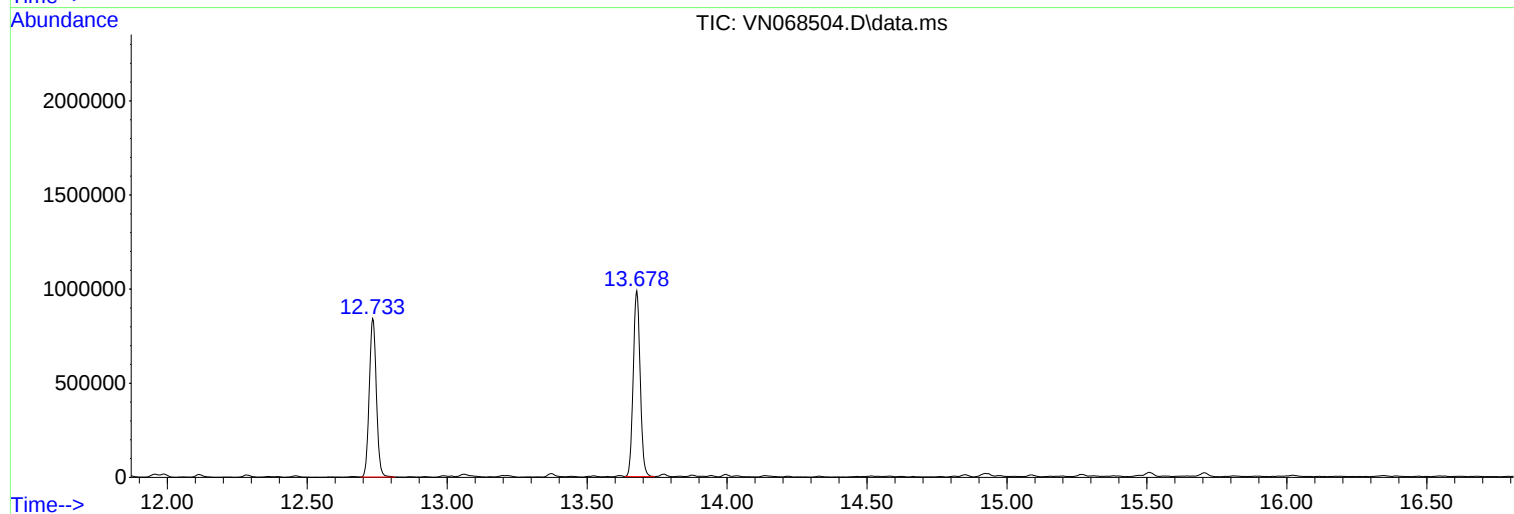
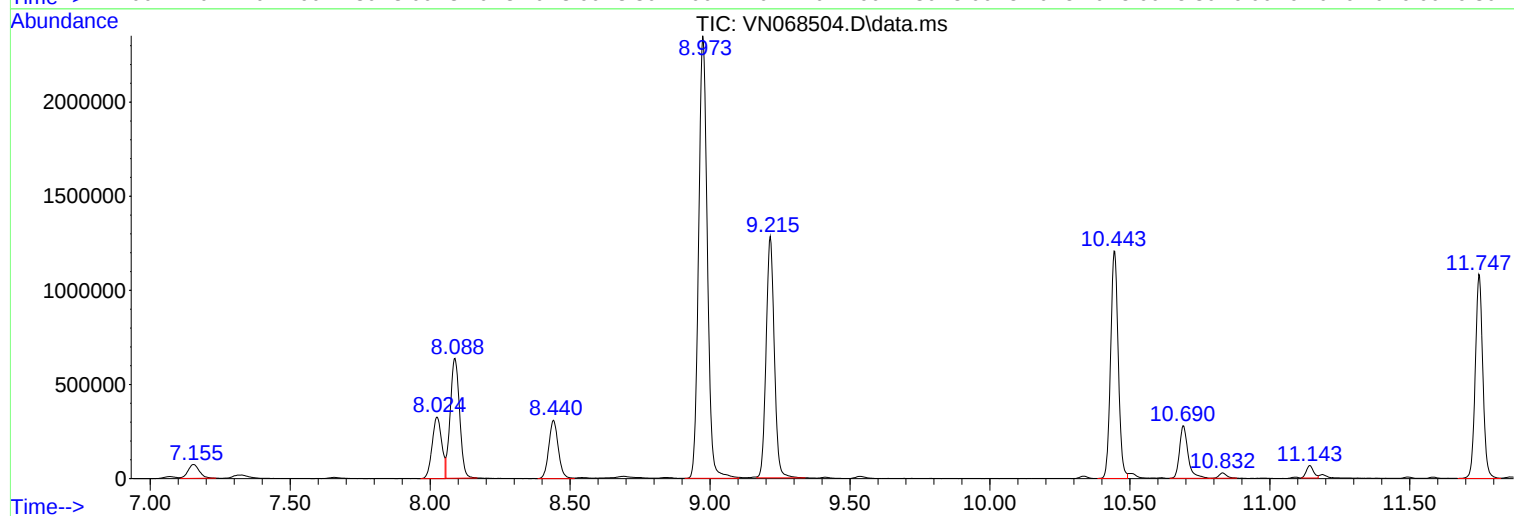
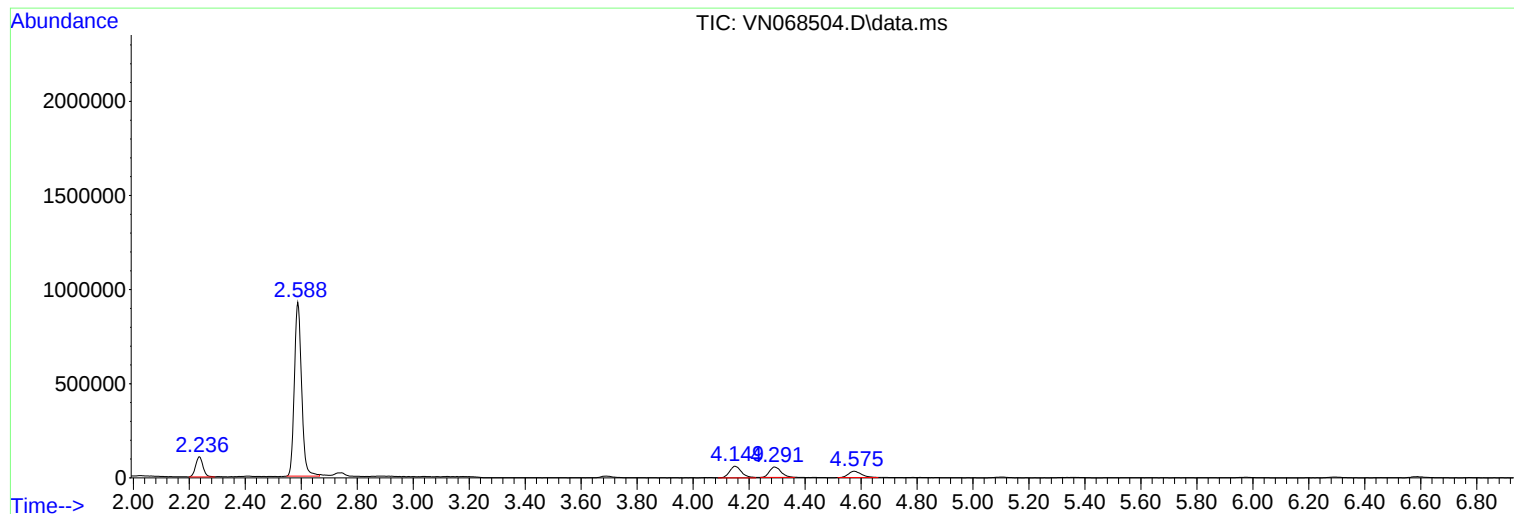
Sum of corrected areas: 21438201

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068504.D
Acq On : 16 Sep 2021 19:10
Operator : JC/MD
Sample : M3759-17 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31185

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068504.D
Acq On : 16 Sep 2021 19:10
Operator : JC/MD
Sample : M3759-17 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31185

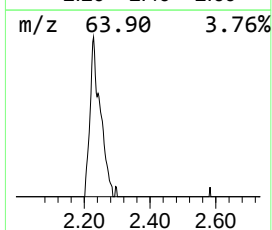
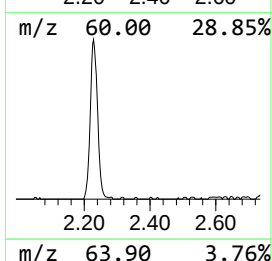
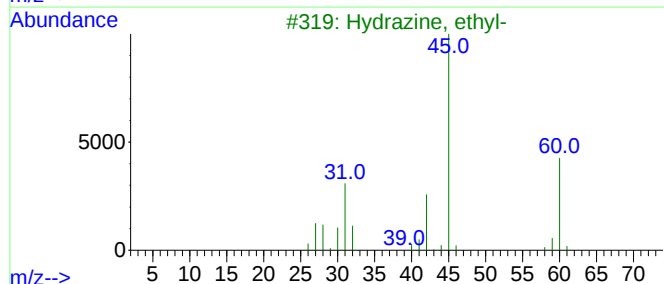
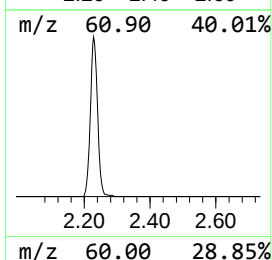
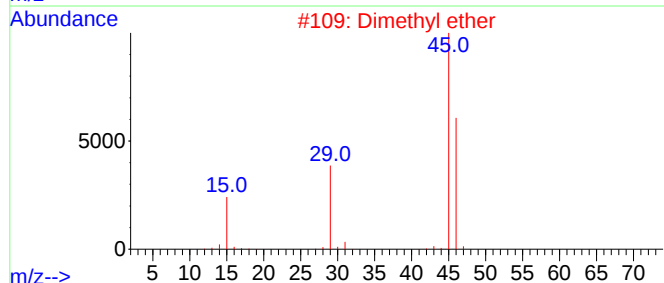
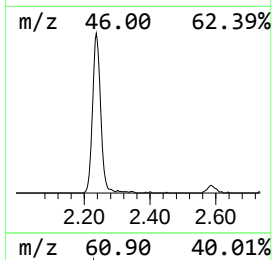
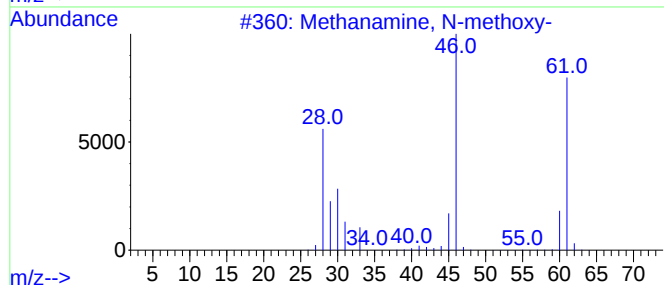
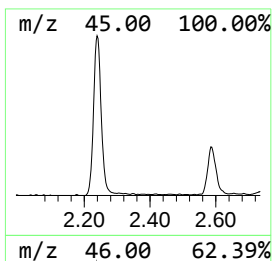
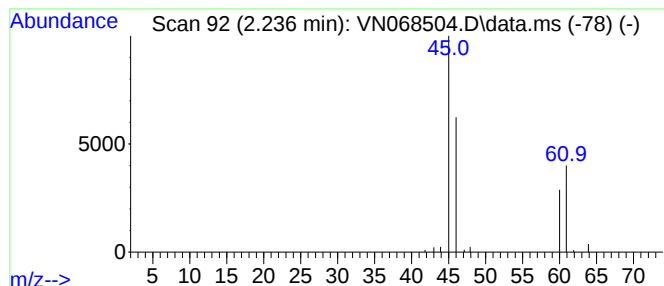
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.236 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.236	6.61 ug/l	192673	Pentafluorobenzene	8.088

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methanamine, N-methoxy-	61	C2H7NO	001117-97-1	32
2		Dimethyl ether	46	C2H6O	000115-10-6	9
3		Hydrazine, ethyl-	60	C2H8N2	000624-80-6	7
4		Ethanol	46	C2H6O	000064-17-5	5
5		Thiirane	60	C2H4S	000420-12-2	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068504.D
Acq On : 16 Sep 2021 19:10
Operator : JC/MD
Sample : M3759-17 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31185

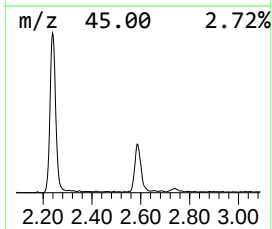
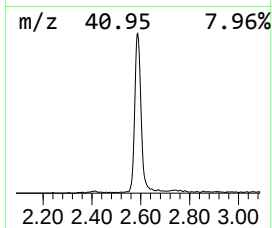
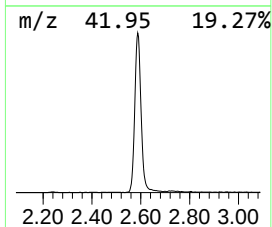
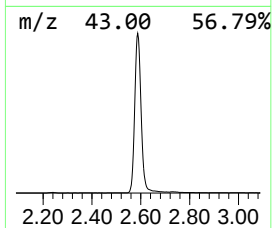
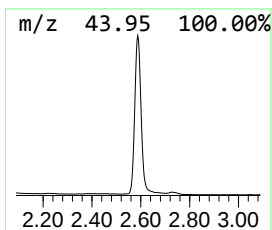
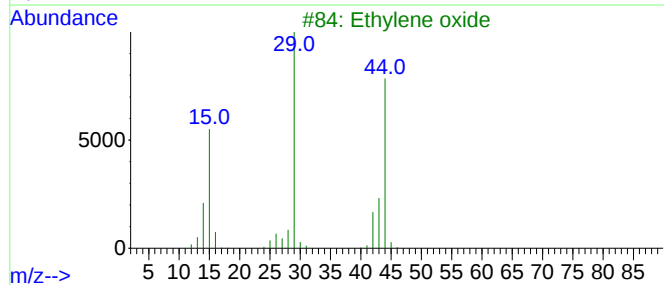
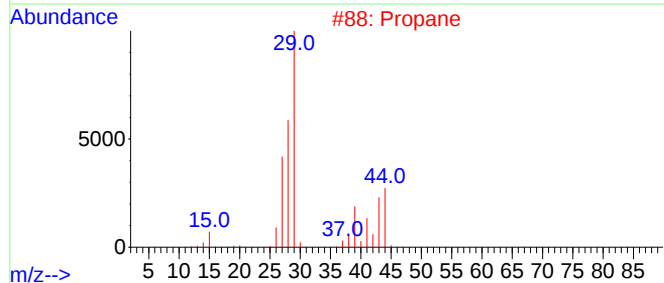
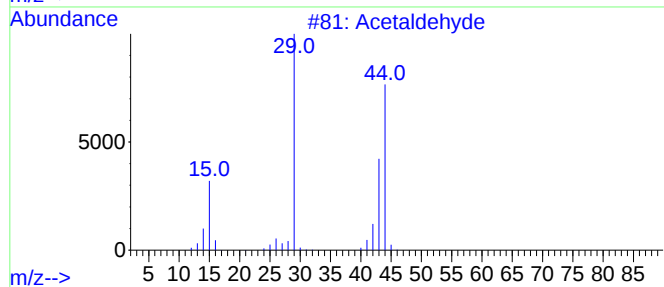
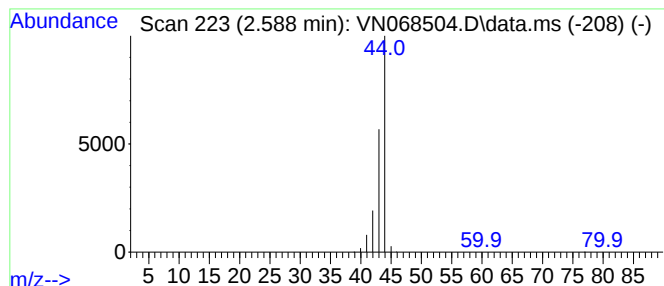
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.588	56.99 ug/l	1661080	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Hydrogen isocyanate	43	CHNO	000075-13-8	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068504.D
Acq On : 16 Sep 2021 19:10
Operator : JC/MD
Sample : M3759-17 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31185

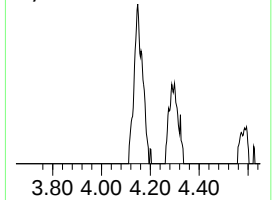
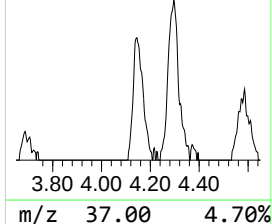
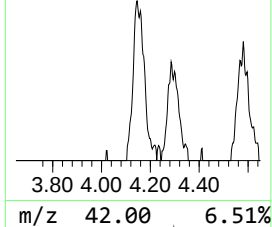
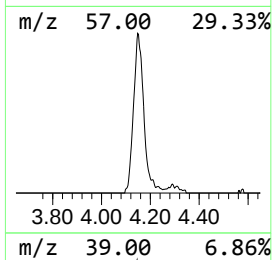
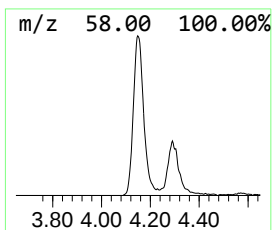
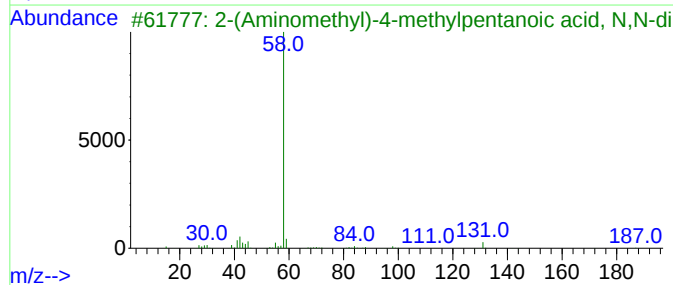
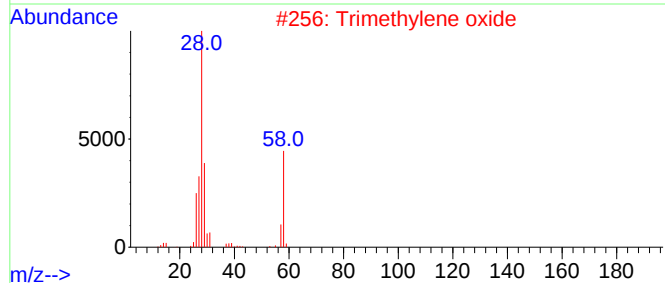
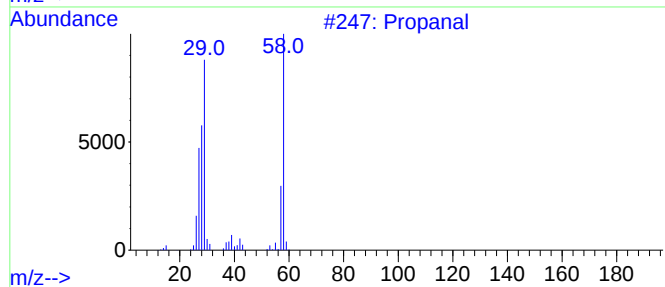
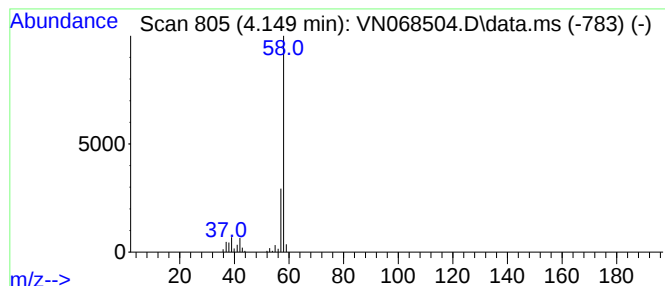
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.149	6.23 ug/l	181503	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	72
2			Trimethylene oxide	58	C3H6O	000503-30-0	50
3			2-(Aminomethyl)-4-methylpentanoic...	187	C10H21NO2	1891211-54-3	9
4			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
5			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068504.D
Acq On : 16 Sep 2021 19:10
Operator : JC/MD
Sample : M3759-17 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31185

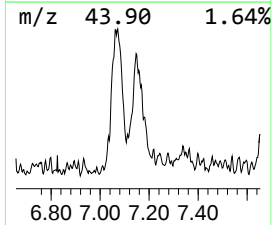
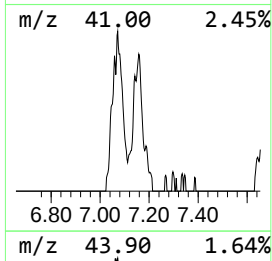
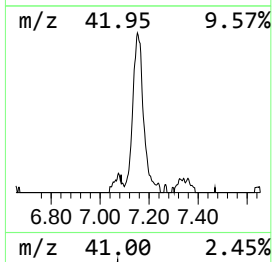
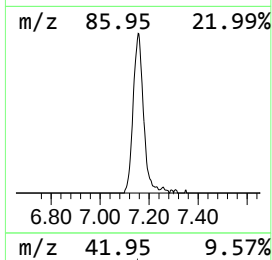
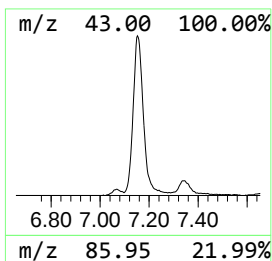
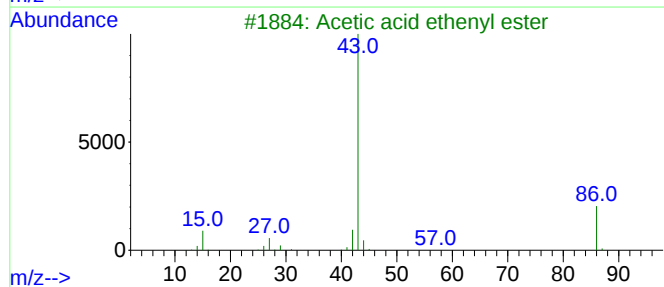
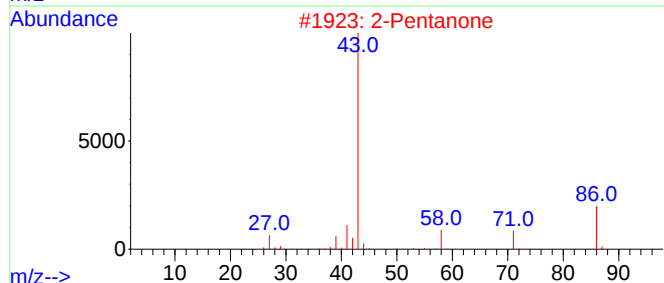
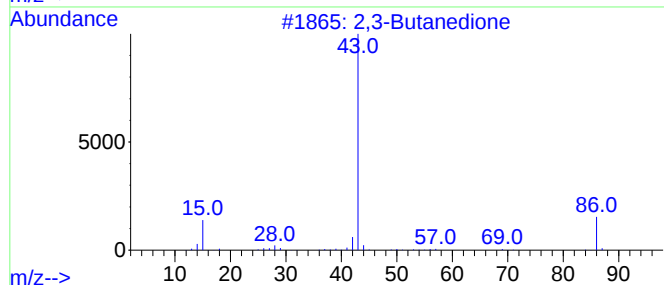
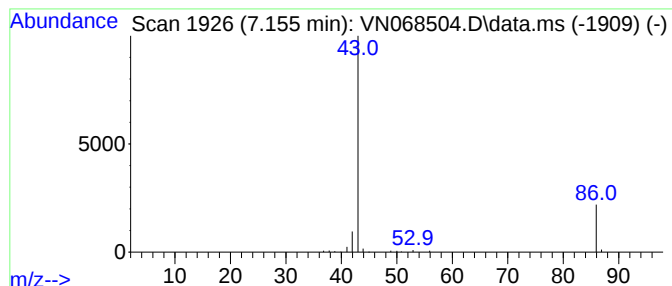
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 4 2,3-Butanedione Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.155	7.01 ug/l	204395	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione			86	C4H6O2	000431-03-8	80
2	2-Pentanone			86	C5H10O	000107-87-9	56
3	Acetic acid ethenyl ester			86	C4H6O2	000108-05-4	9
4	Ethanone, 1-oxiranyl-			86	C4H6O2	004401-11-0	5
5	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068504.D
Acq On : 16 Sep 2021 19:10
Operator : JC/MD
Sample : M3759-17 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31185

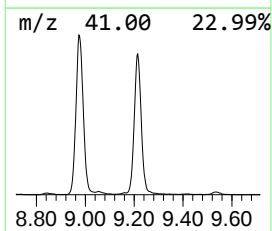
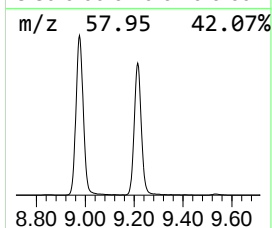
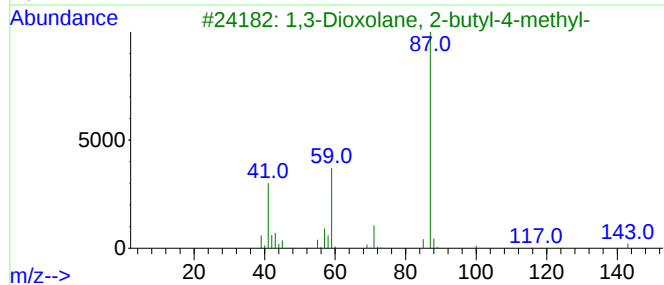
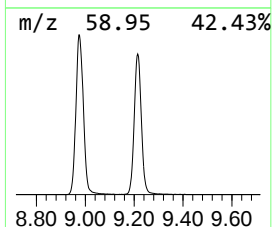
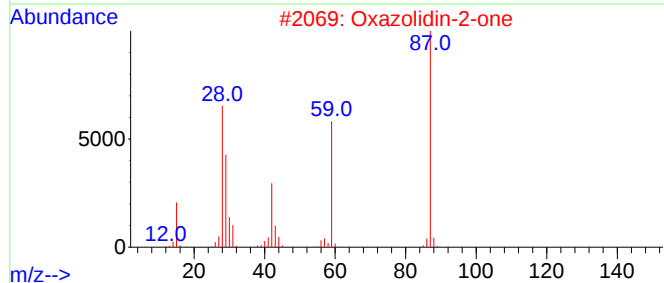
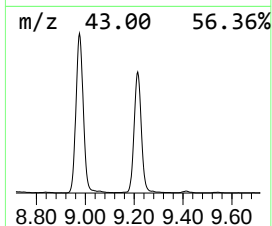
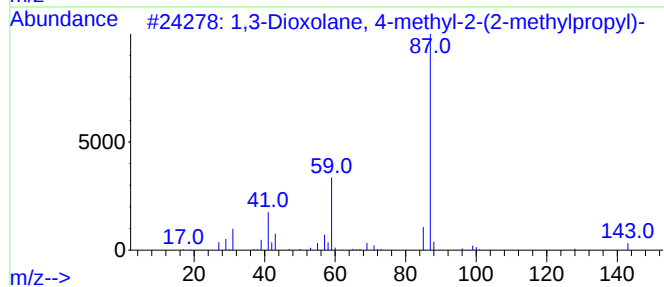
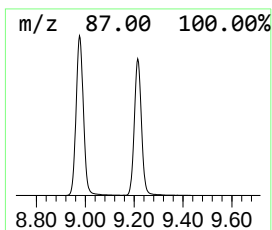
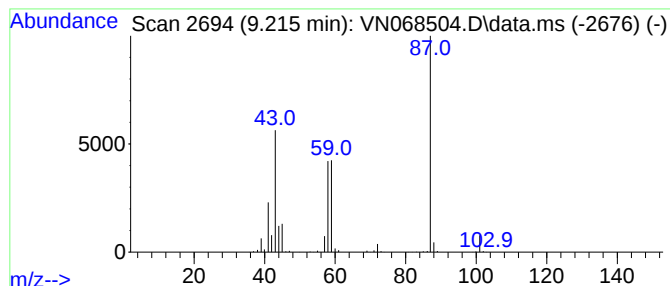
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 5 1,3-Dioxolane, 4-methyl-2-(... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.215	25.66 ug/l	2602770	1,4-Difluorobenzene	8.971

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	50
2		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
3		1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	36
4		1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	33
5		1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068504.D
Acq On : 16 Sep 2021 19:10
Operator : JC/MD
Sample : M3759-17 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31185

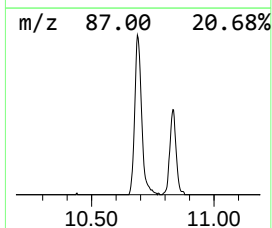
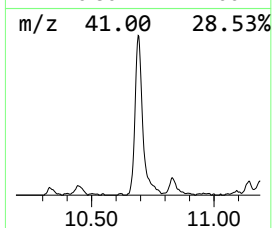
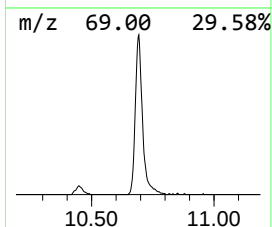
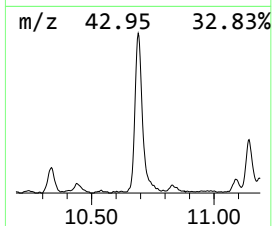
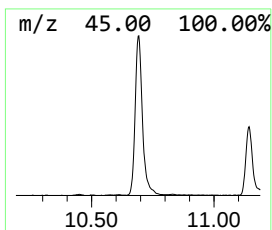
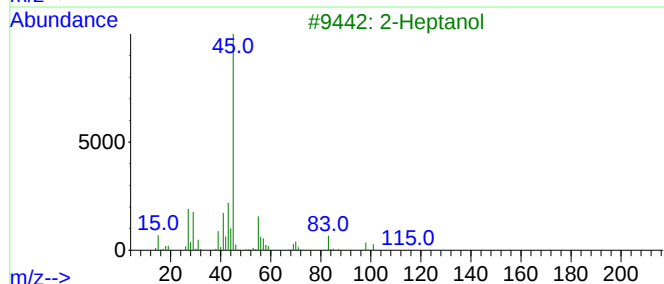
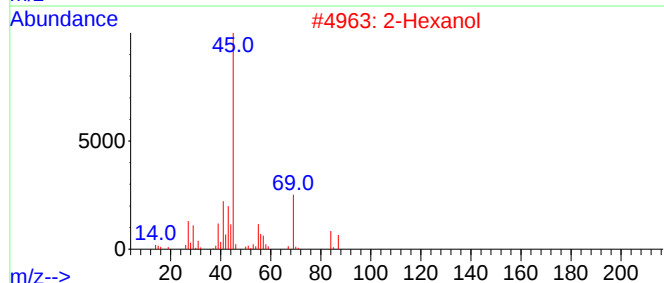
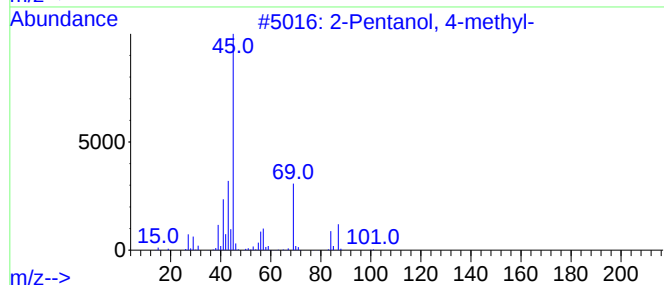
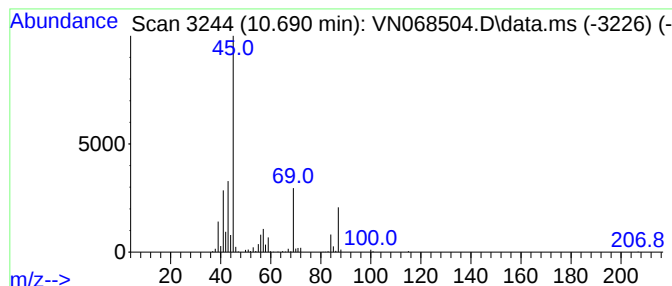
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 6 2-Pentanol, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.690	14.57 ug/l	589620	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-			102	C6H14O	000108-11-2	80
2	2-Hexanol			102	C6H14O	000626-93-7	59
3	2-Heptanol			116	C7H16O	000543-49-7	59
4	1-Butene, 4-methoxy			86	C5H10O	004696-30-4	50
5	2-Nonanol			144	C9H20O	000628-99-9	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068504.D
Acq On : 16 Sep 2021 19:10
Operator : JC/MD
Sample : M3759-17 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31185

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.236	2.236	6.6	ug/l	192673	1	8.088	1457390	50.0
Acetaldehyde	2.588	57.0	ug/l	1661080	1	8.088	1457390	50.0
Propanal	4.149	6.2	ug/l	181503	1	8.088	1457390	50.0
2,3-Butanedione	7.155	7.0	ug/l	204395	1	8.088	1457390	50.0
1,3-Dioxolane, ...	9.215	25.7	ug/l	2602770	2	8.971	5070950	50.0
2-Pentanol, 4-m...	10.690	14.6	ug/l	589620	3	11.746	2023700	50.0