

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101022\
 Data File : VN074836.D
 Acq On : 10 Oct 2022 17:01
 Operator : JC\MD
 Sample : N5042-03 50X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 EOR-0615

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\82N100522W.M

Title : SW846 8260

Signal : TIC: VN074836.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.312	37	44	50	rBV	207940	409632	1.01%	0.455%
2	2.683	101	107	116	rBV	429806	793489	1.95%	0.880%
3	3.824	292	301	314	rBV2	270420	722430	1.78%	0.802%
4	4.312	373	384	397	rBV	2031440	5906900	14.55%	6.555%
5	4.453	397	408	430	rVV	5187465	15605587	38.43%	17.317%
6	4.742	446	457	485	rVB	2348772	7755079	19.10%	8.605%
7	6.789	783	805	829	rBV	12752645	40606709	100.00%	45.059%
8	8.177	1032	1041	1046	rBV	505979	1237266	3.05%	1.373%
9	8.236	1046	1051	1062	rVB	579325	1259445	3.10%	1.398%
10	8.588	1097	1111	1124	rBV2	633717	1473350	3.63%	1.635%
11	9.106	1190	1199	1211	rBV	801662	1682393	4.14%	1.867%
12	10.571	1440	1448	1456	rBV	2228444	4063784	10.01%	4.509%
13	10.806	1479	1488	1498	rVB2	288763	547505	1.35%	0.608%
14	11.206	1548	1556	1564	rBV	471605	769566	1.90%	0.854%
15	11.835	1656	1663	1664	rBV2	333341	519076	1.28%	0.576%
16	11.871	1664	1669	1680	rVB	1269406	2350714	5.79%	2.608%
17	12.853	1825	1836	1847	rBV	1253200	2208172	5.44%	2.450%
18	13.794	1987	1996	2005	rBV	1274847	2207482	5.44%	2.450%

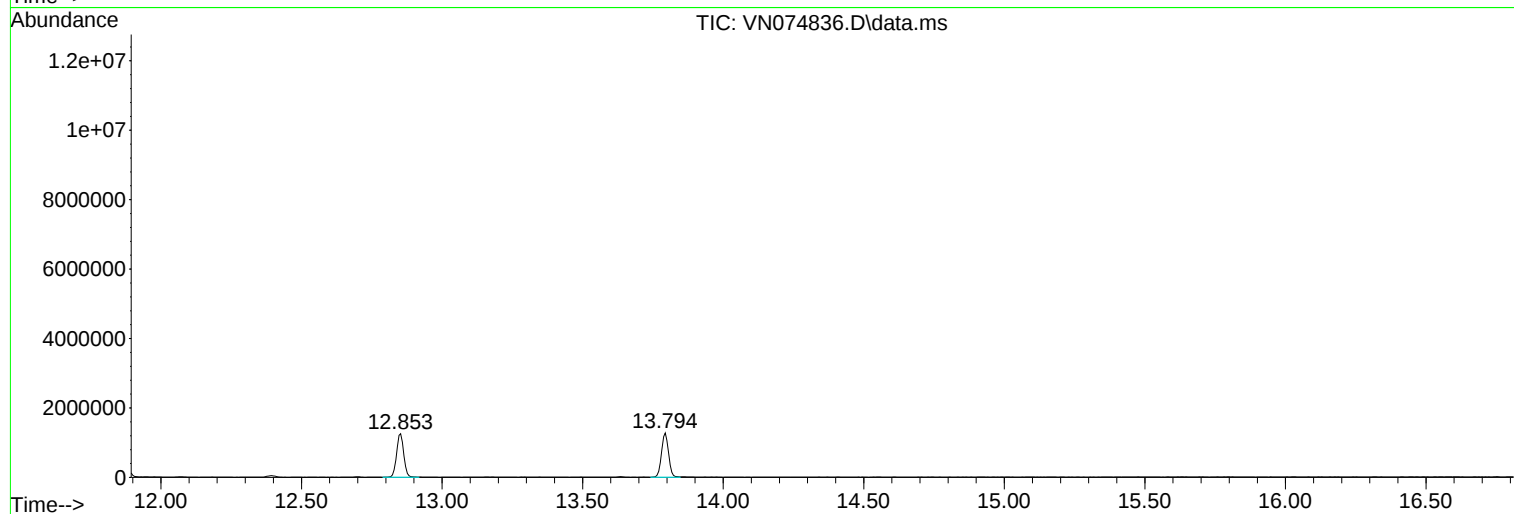
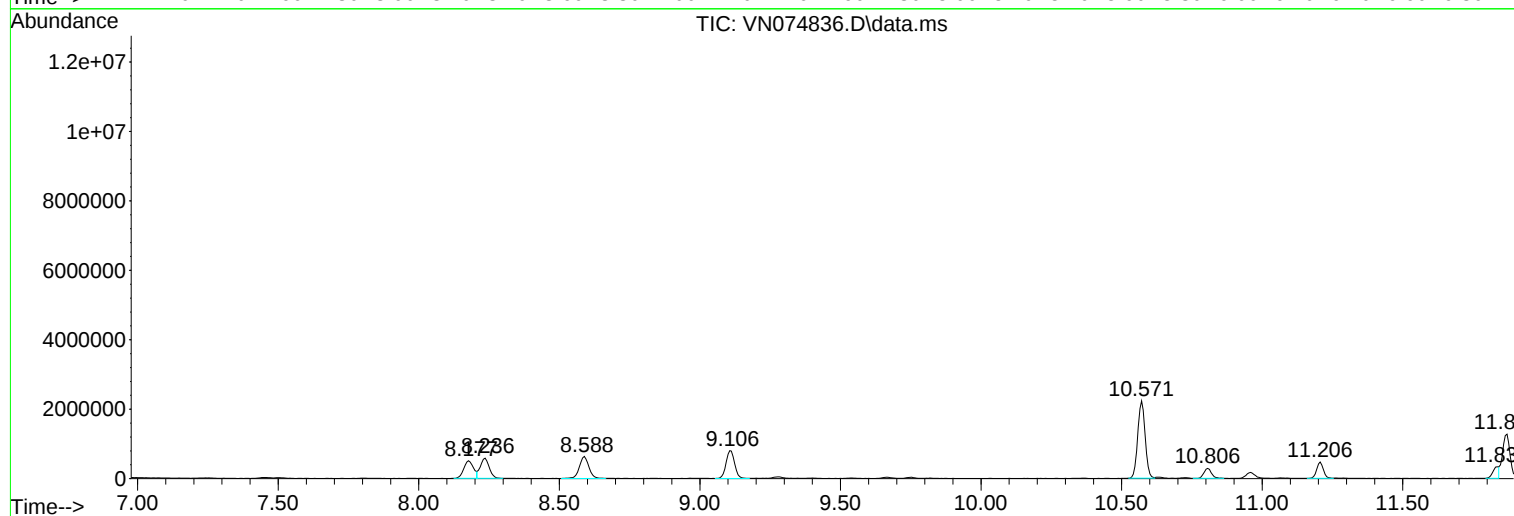
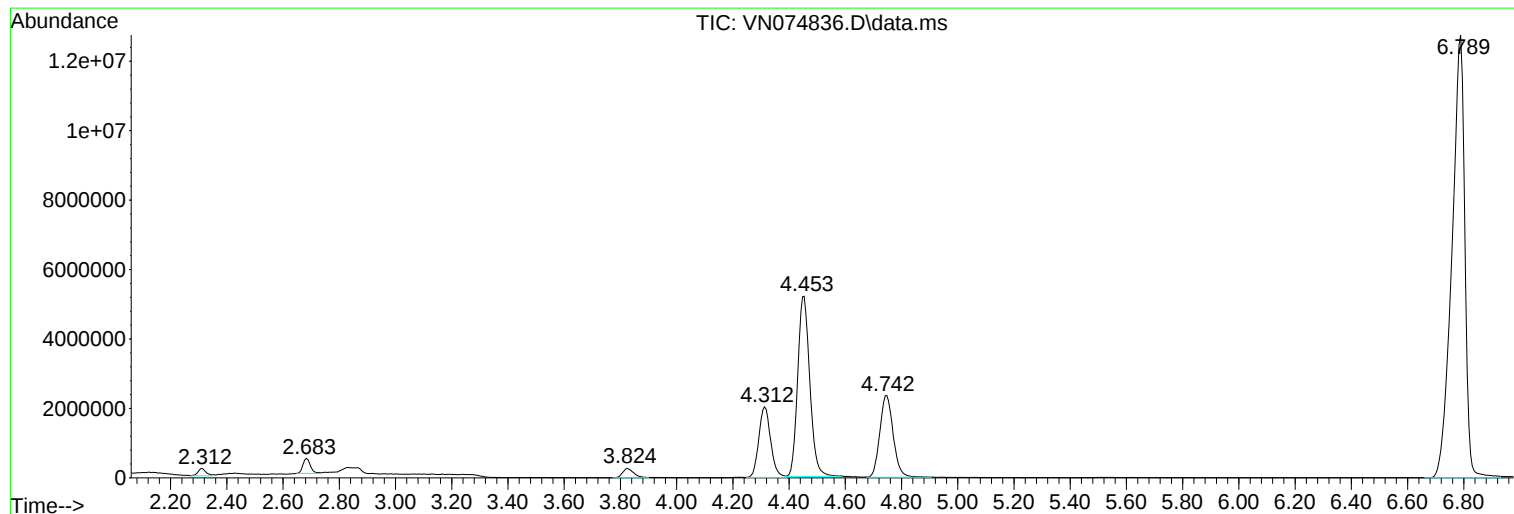
Sum of corrected areas: 90118579

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101022\
Data File : VN074836.D
Acq On : 10 Oct 2022 17:01
Operator : JC\MD
Sample : N5042-03 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EOR-0615

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101022\
Data File : VN074836.D
Acq On : 10 Oct 2022 17:01
Operator : JC\MD
Sample : N5042-03 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

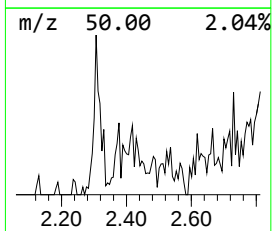
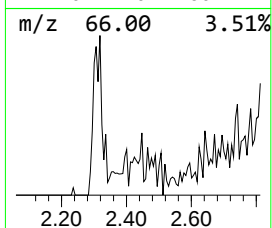
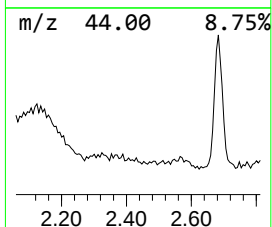
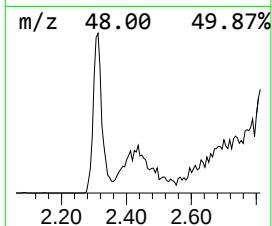
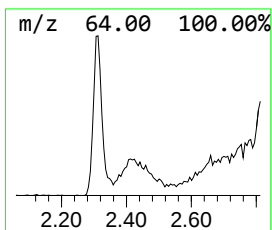
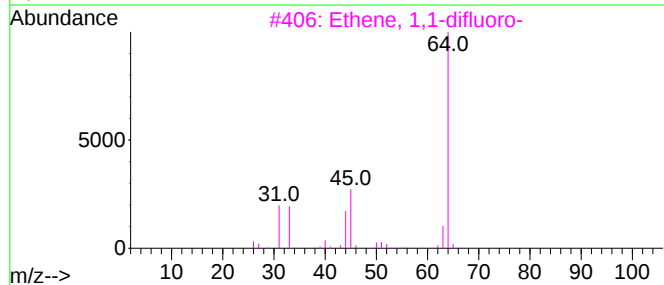
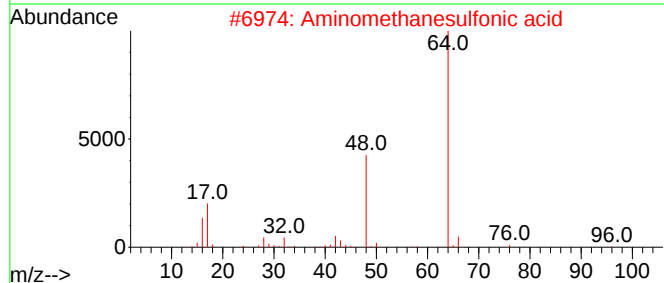
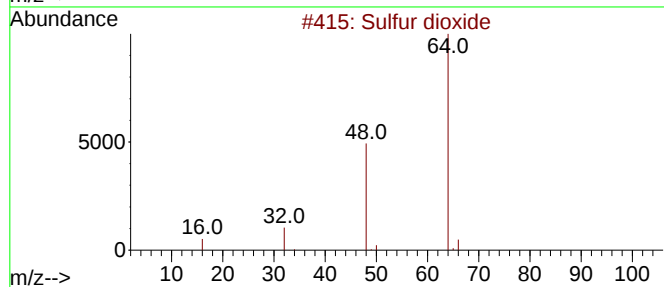
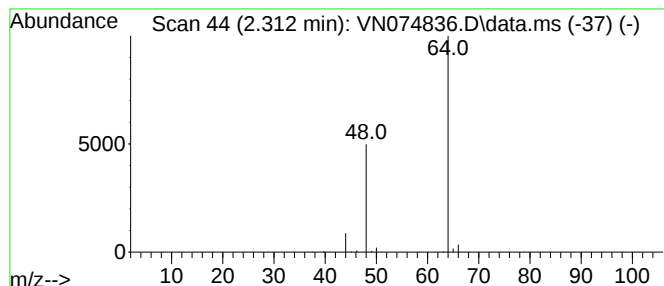
Instrument :
MSVOA_N
ClientSampleId :
EOR-0615

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.312	16.26 ug/l	409632	Pentafluorobenzene	8.230	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101022\
Data File : VN074836.D
Acq On : 10 Oct 2022 17:01
Operator : JC\MD
Sample : N5042-03 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EOR-0615

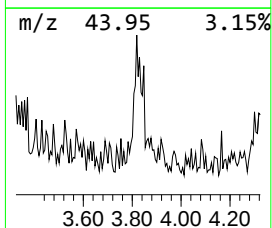
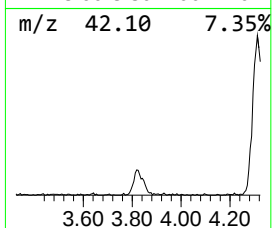
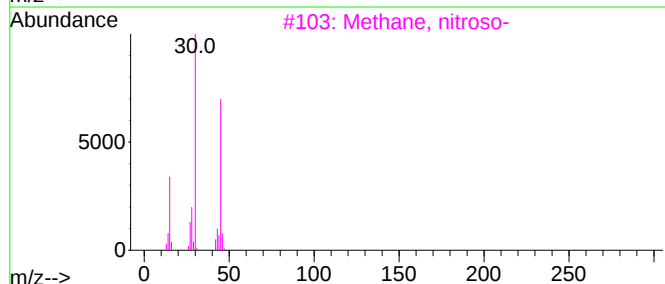
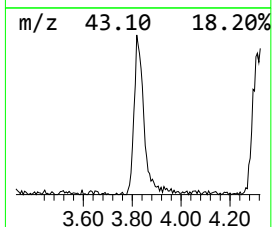
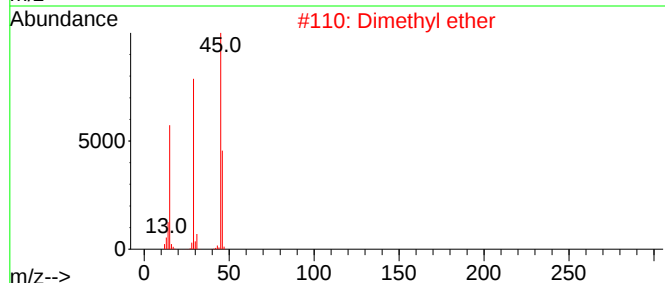
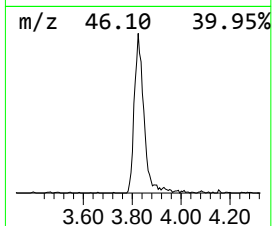
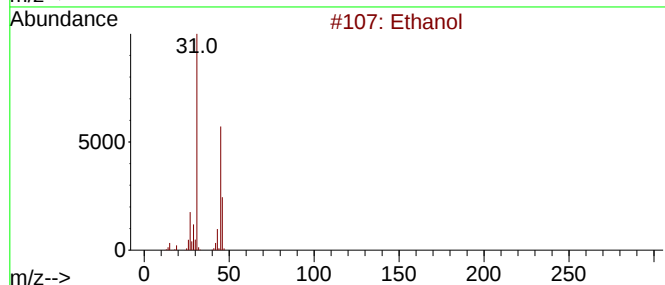
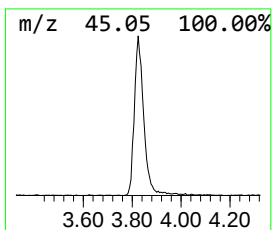
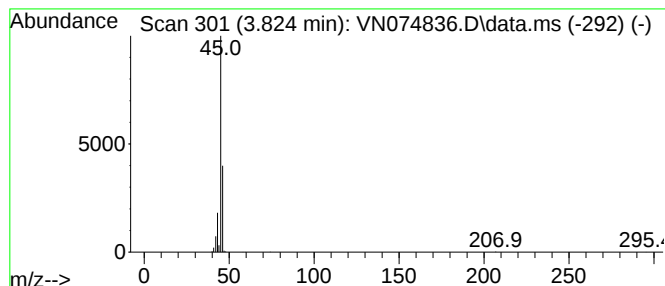
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.824	28.68 ug/l	722430	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	64
2	Dimethyl ether			46	C2H6O	000115-10-6	5
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Formic acid			46	CH2O2	000064-18-6	4
5	Oxalic acid			90	C2H2O4	000144-62-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101022\
Data File : VN074836.D
Acq On : 10 Oct 2022 17:01
Operator : JC\MD
Sample : N5042-03 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EOR-0615

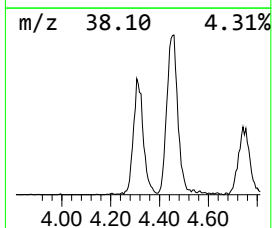
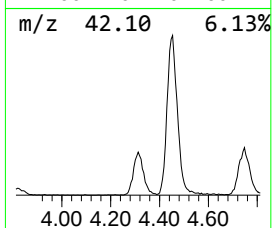
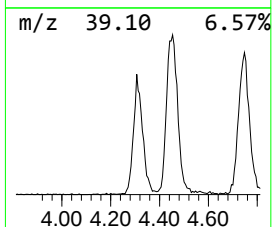
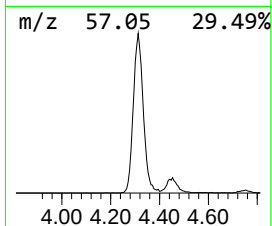
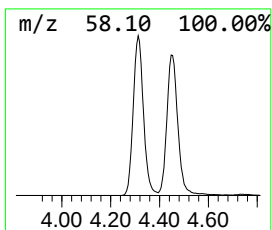
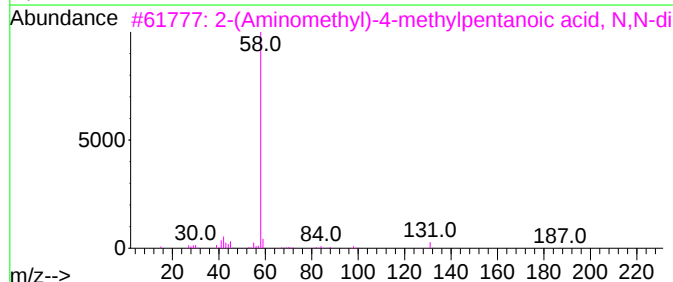
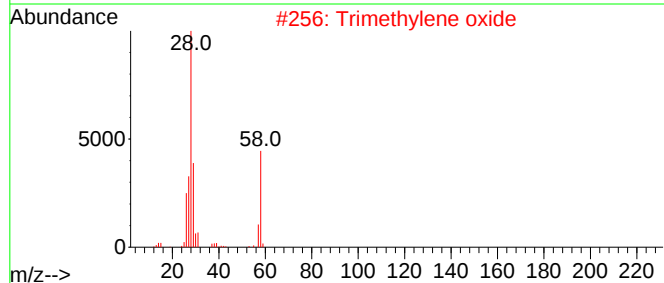
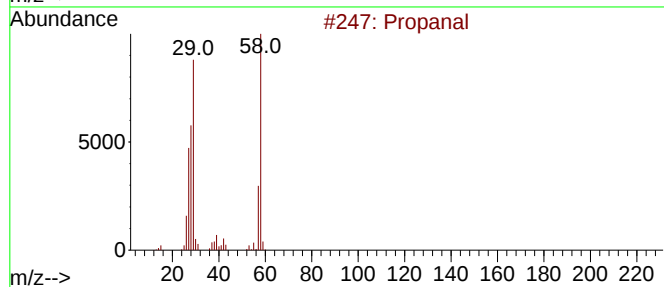
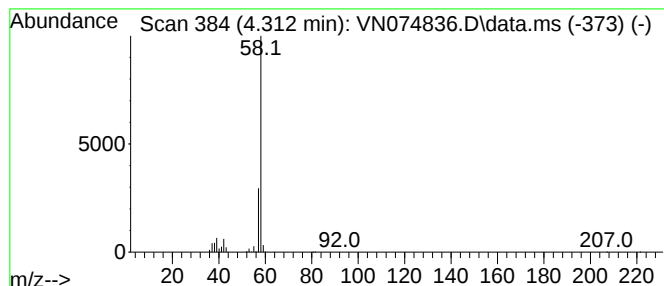
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 4 Propanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	234.50 ug/l	5906900	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	56
3			2-(Aminomethyl)-4-methylpentanoic...	187	C10H21NO2	1891211-54-3	9
4			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
5			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101022\
Data File : VN074836.D
Acq On : 10 Oct 2022 17:01
Operator : JC\MD
Sample : N5042-03 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EOR-0615

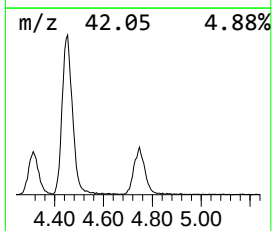
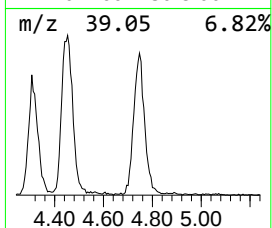
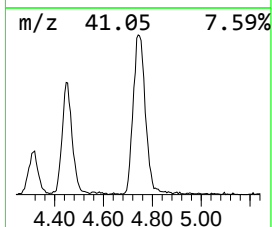
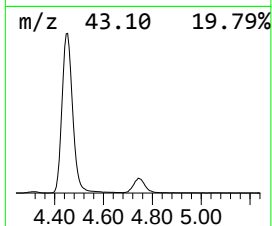
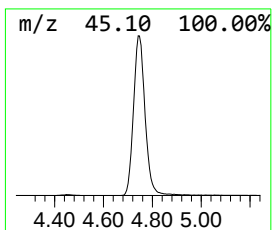
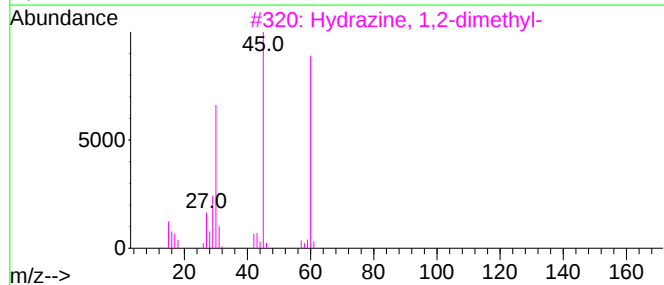
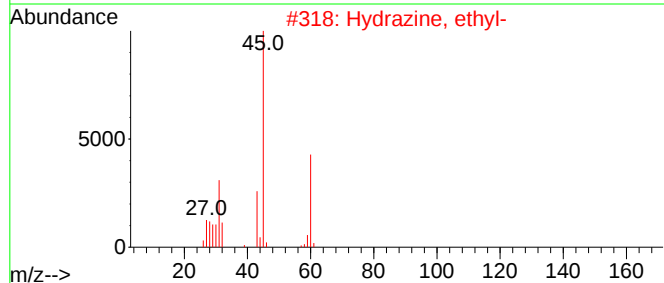
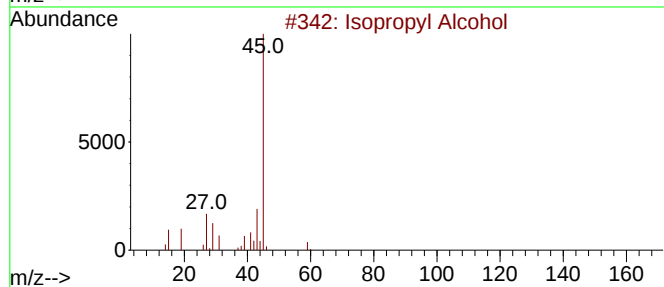
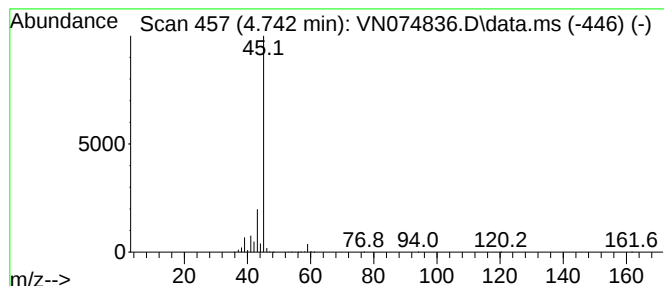
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 5 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.742	307.88 ug/l	7755080	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4			Formamide	45	CH3NO	000075-12-7	4
5			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101022\
Data File : VN074836.D
Acq On : 10 Oct 2022 17:01
Operator : JC\MD
Sample : N5042-03 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EOR-0615

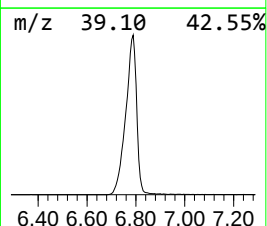
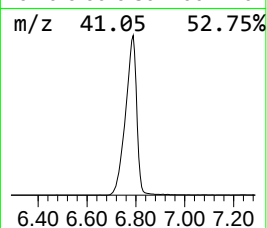
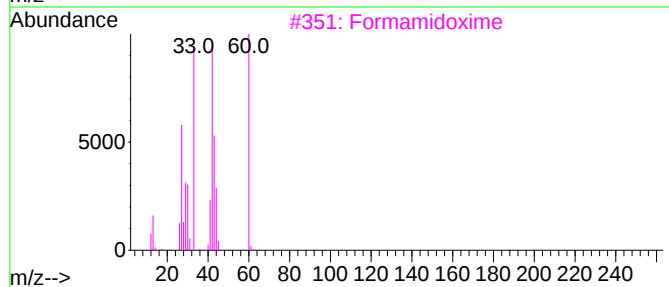
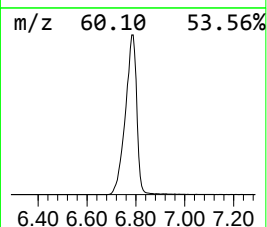
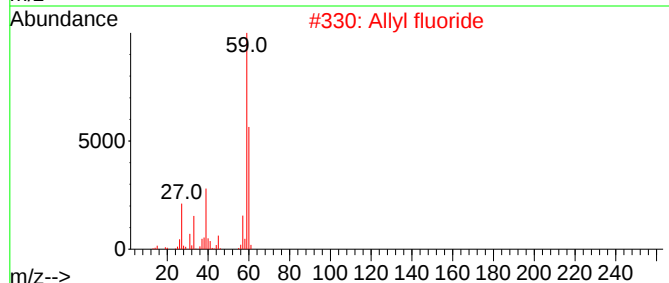
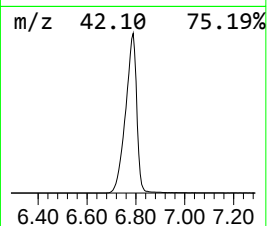
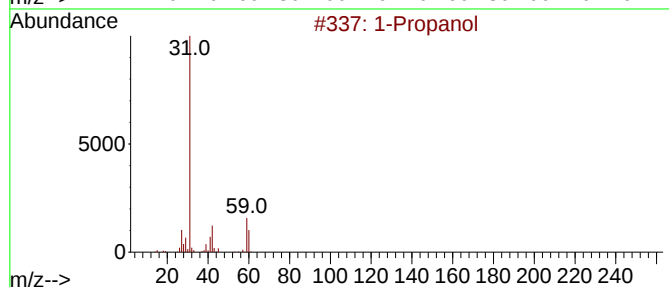
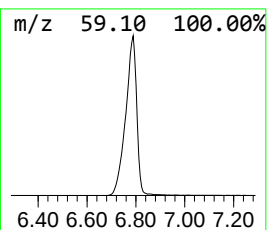
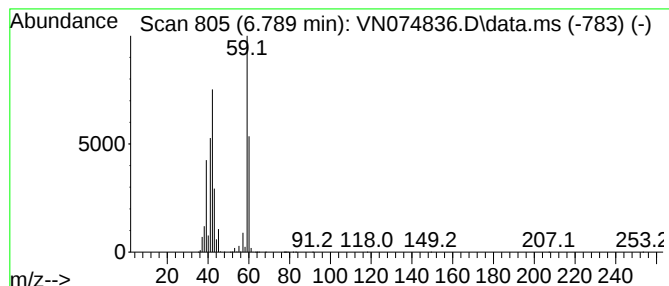
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 6 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.789	1612.09 ug/l	40606700	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	64
2			Allyl fluoride	60	C3H5F	000818-92-8	38
3			Formamidoxime	60	CH4N2O	000624-82-8	35
4			Cyclopropane	42	C3H6	000075-19-4	32
5			2-Fluoropropene	60	C3H5F	001184-60-7	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101022\
Data File : VN074836.D
Acq On : 10 Oct 2022 17:01
Operator : JC\MD
Sample : N5042-03 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

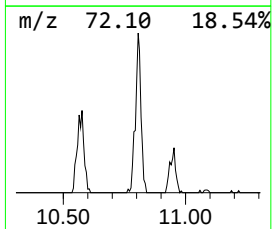
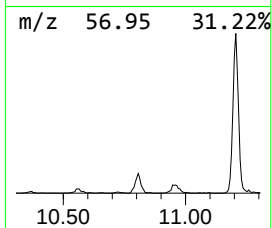
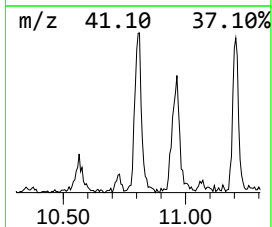
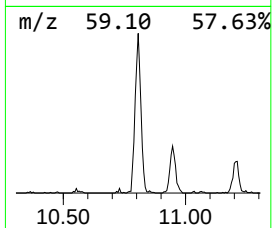
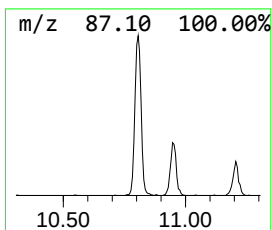
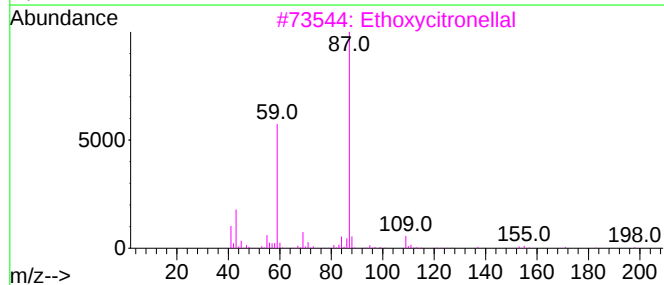
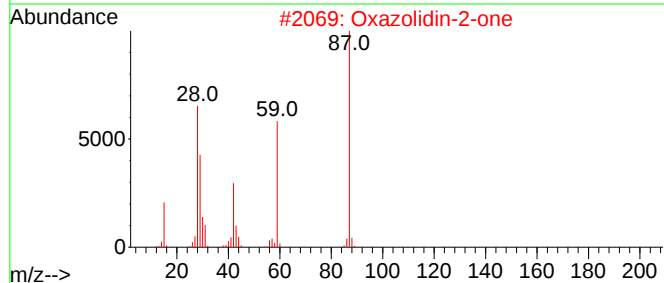
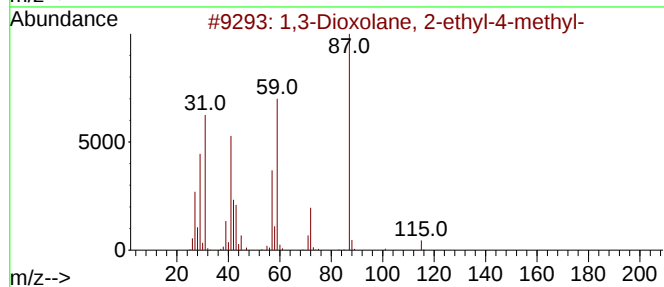
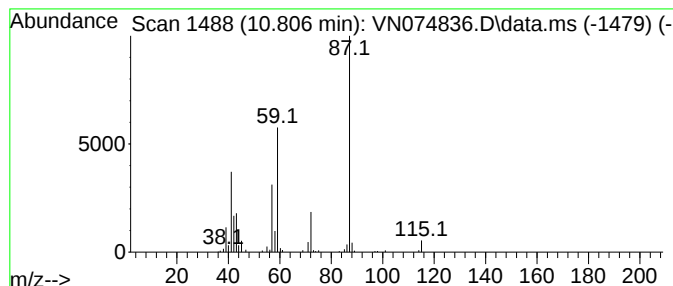
Instrument :
MSVOA_N
ClientSampleId :
EOR-0615

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 7 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.806	11.65 ug/l	547505	Chlorobenzene-d5	11.871	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	90
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
3	Ethoxycitronellal	198	C12H22O2	1000132-02-6	59
4	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	50
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101022\
Data File : VN074836.D
Acq On : 10 Oct 2022 17:01
Operator : JC\MD
Sample : N5042-03 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EOR-0615

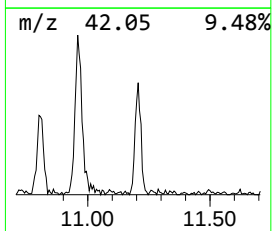
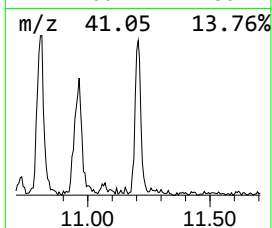
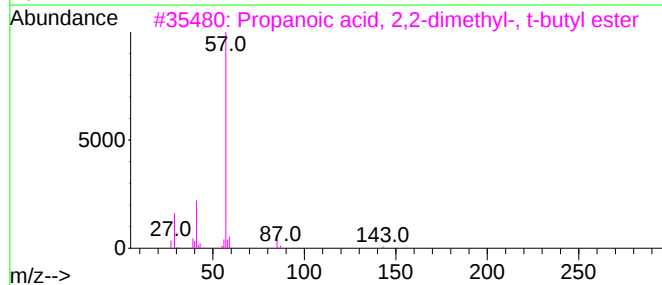
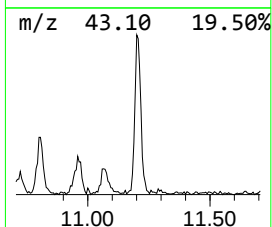
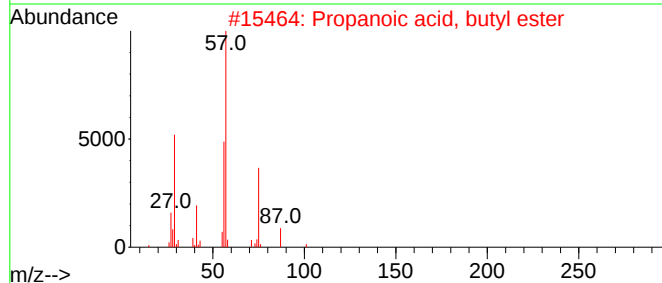
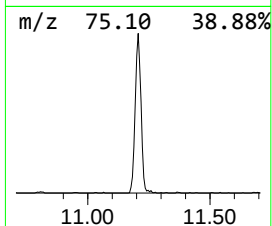
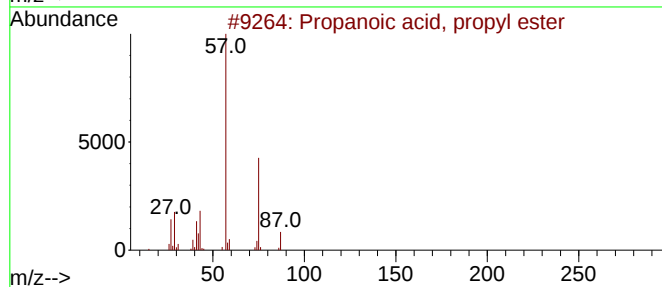
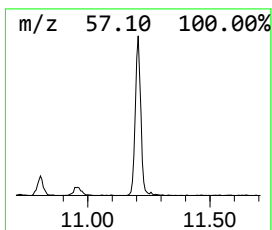
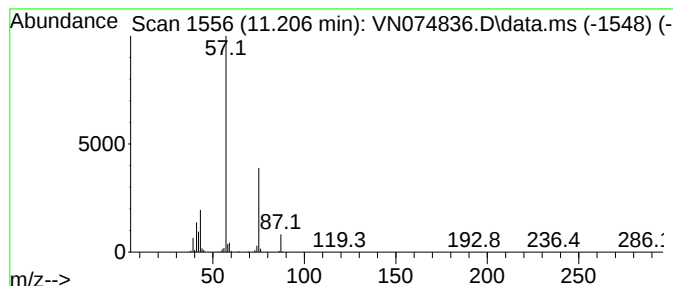
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 8 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	16.37 ug/l	769566	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38
3			Propanoic acid, 2,2-dimethyl-, t...	158	C9H18O2	016474-43-4	9
4			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5			Azetidine	57	C3H7N	000503-29-7	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101022\
Data File : VN074836.D
Acq On : 10 Oct 2022 17:01
Operator : JC\MD
Sample : N5042-03 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EOR-0615

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.312	16.3	ug/l	409632	1	8.230	1259450	50.0
Ethanol	3.824	28.7	ug/l	722430	1	8.230	1259450	50.0
Propanal	4.312	234.5	ug/l	5906900	1	8.230	1259450	50.0
Isopropyl Alcohol	4.742	307.9	ug/l	7755080	1	8.230	1259450	50.0
1-Propanol	6.789	1612.1	ug/l	40606700	1	8.230	1259450	50.0
1,3-Dioxolane, ...	10.806	11.7	ug/l	547505	3	11.871	2350710	50.0
Propanoic acid,...	11.206	16.4	ug/l	769566	3	11.871	2350710	50.0