

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
 Data File : VN065305.D
 Acq On : 29 Dec 2020 14:46
 Operator : JC/MD
 Sample : L5226-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 16882

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\82N122220W.M

Title : Sw846 8260

Signal : TIC: VN065305.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.142	115	125	136	rBV	41975	60818	1.26%	0.356%
2	2.296	160	173	218	rBV	1598215	2633072	54.41%	15.401%
3	3.254	458	471	490	rVB	26638	61388	1.27%	0.359%
4	3.666	585	599	619	rVB	33489	83271	1.72%	0.487%
5	3.785	624	636	657	rVB	29461	74860	1.55%	0.438%
6	4.775	923	944	972	rBV2	30689	106942	2.21%	0.625%
7	5.370	1107	1129	1162	rVB2	41921	142608	2.95%	0.834%
8	6.502	1458	1481	1547	rBV	1596138	4839704	100.00%	28.307%
9	7.553	1789	1808	1819	rBV	182744	463278	9.57%	2.710%
10	7.627	1819	1831	1852	rVB	365073	866829	17.91%	5.070%
11	7.991	1926	1944	1966	rBV	216685	509699	10.53%	2.981%
12	8.550	2103	2118	2141	rVB	498101	1037264	21.43%	6.067%
13	8.766	2169	2185	2205	rBV	83673	184838	3.82%	1.081%
14	9.135	2282	2300	2324	rBV	102488	208910	4.32%	1.222%
15	10.061	2571	2588	2626	rBV	780149	1469061	30.35%	8.592%
16	11.380	2985	2998	3025	rVB	754396	1330696	27.50%	7.783%
17	11.974	3175	3183	3206	rVB	24447	49801	1.03%	0.291%
18	12.376	3294	3308	3334	rBV	550865	944993	19.53%	5.527%
19	12.888	3457	3467	3485	rVB	84287	134179	2.77%	0.785%
20	13.080	3518	3527	3544	rVB	34789	63618	1.31%	0.372%
21	13.174	3545	3556	3565	rBV2	34545	59334	1.23%	0.347%
22	13.318	3588	3601	3621	rBV	597515	1023512	21.15%	5.986%
23	13.425	3622	3634	3652	rBV	443388	748448	15.46%	4.378%

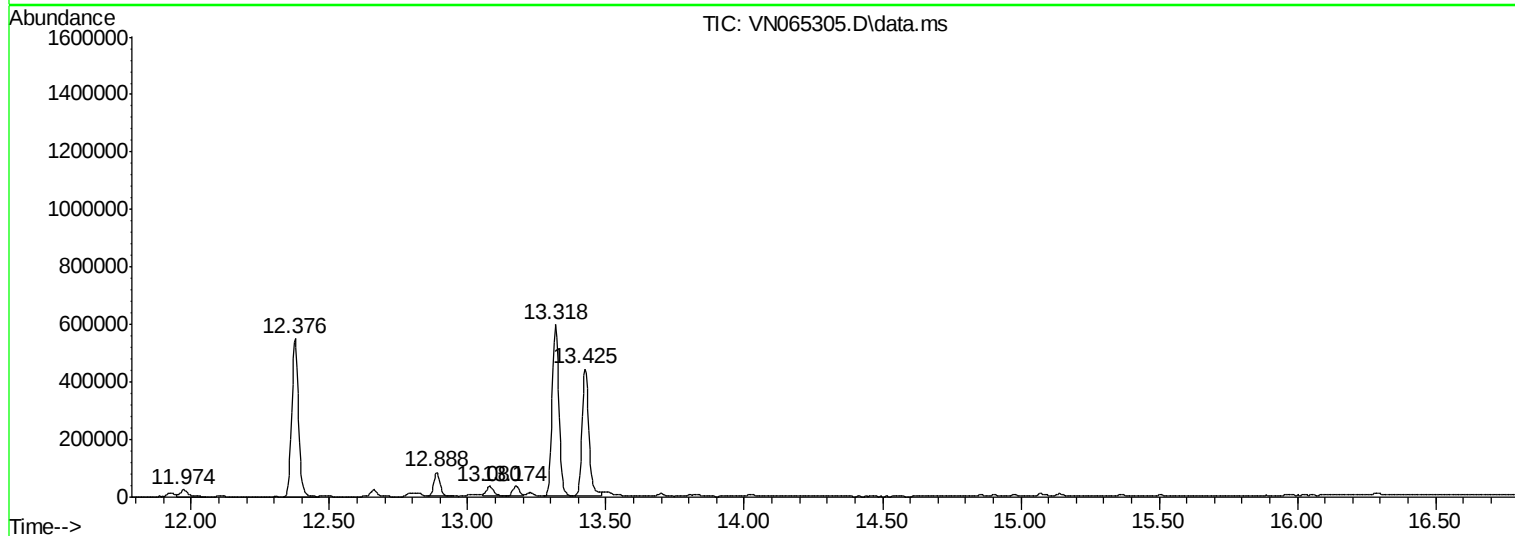
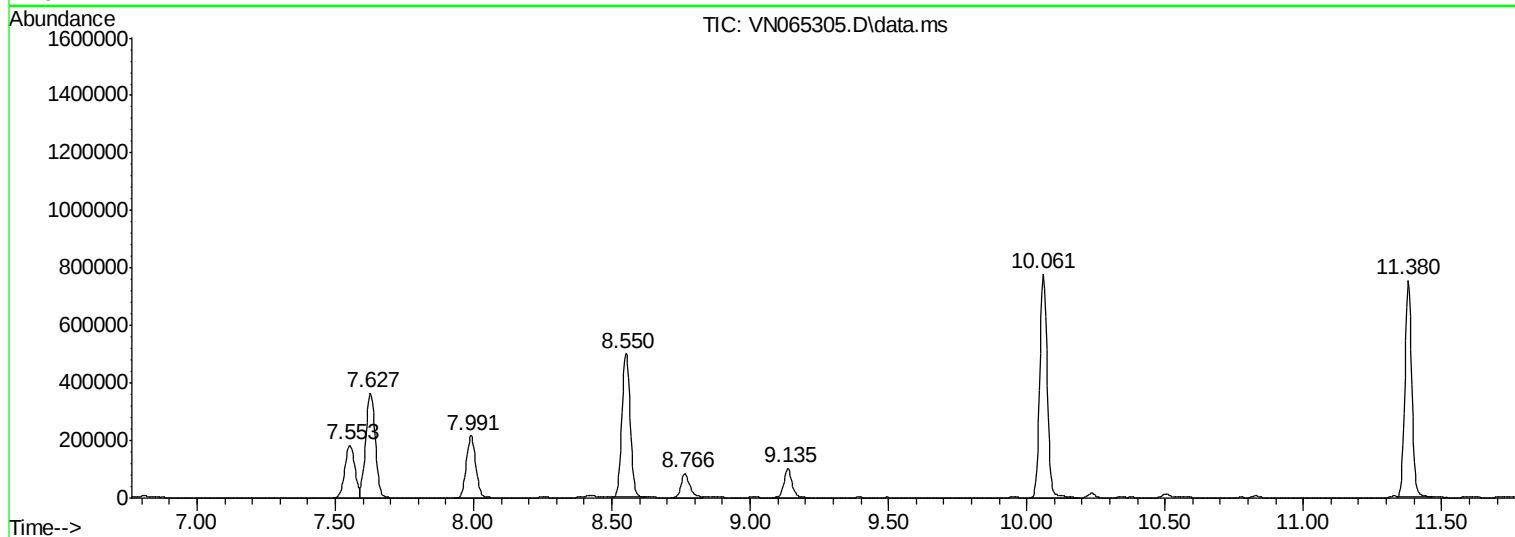
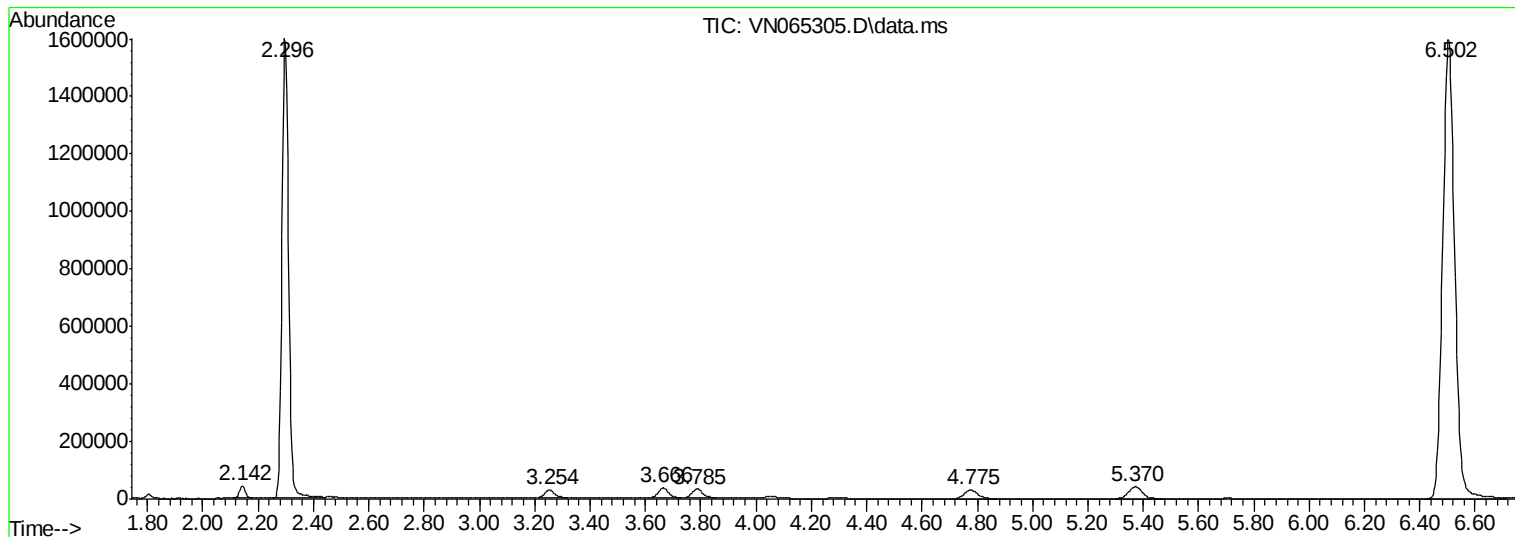
Sum of corrected areas: 17097123

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065305.D
Acq On : 29 Dec 2020 14:46
Operator : JC/MD
Sample : L5226-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
16882

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065305.D
Acq On : 29 Dec 2020 14:46
Operator : JC/MD
Sample : L5226-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
16882

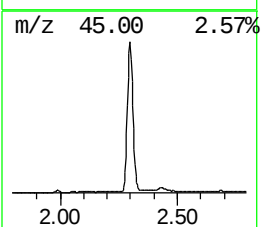
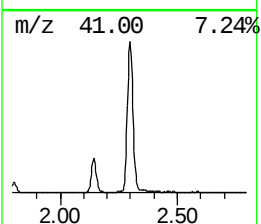
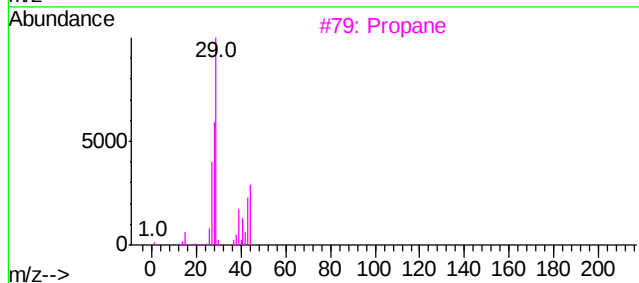
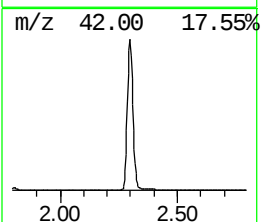
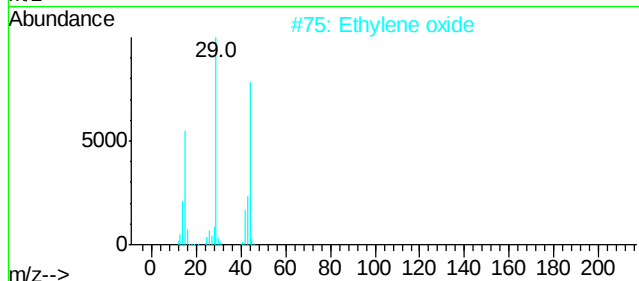
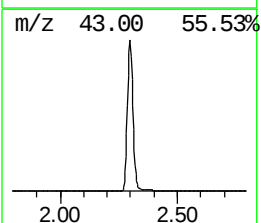
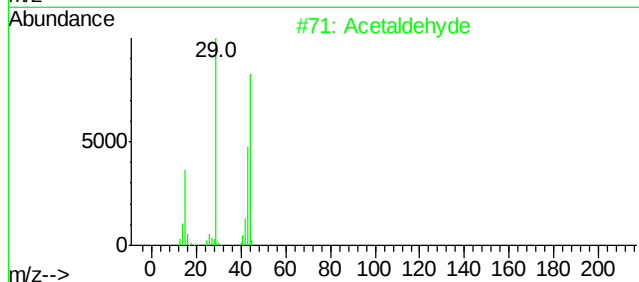
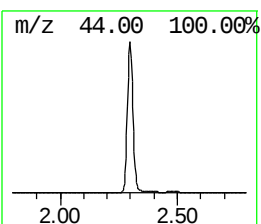
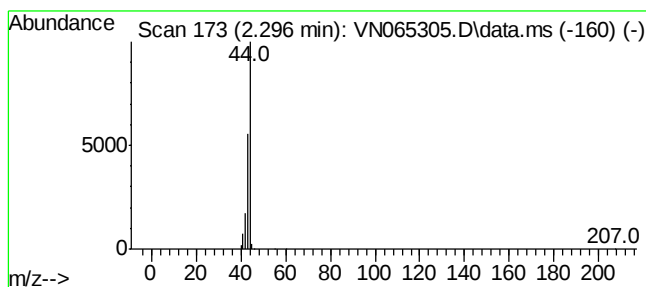
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.296	151.88 ug/l	2633070	Pentafluorobenzene	7.627

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Ethylene oxide	44	C2H4O	000075-21-8	5
3	Propane	44	C3H8	000074-98-6	4
4	1,2-Propanediamine	74	C3H10N2	000078-90-0	4
5	Alanine	89	C3H7NO2	000056-41-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065305.D
Acq On : 29 Dec 2020 14:46
Operator : JC/MD
Sample : L5226-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
16882

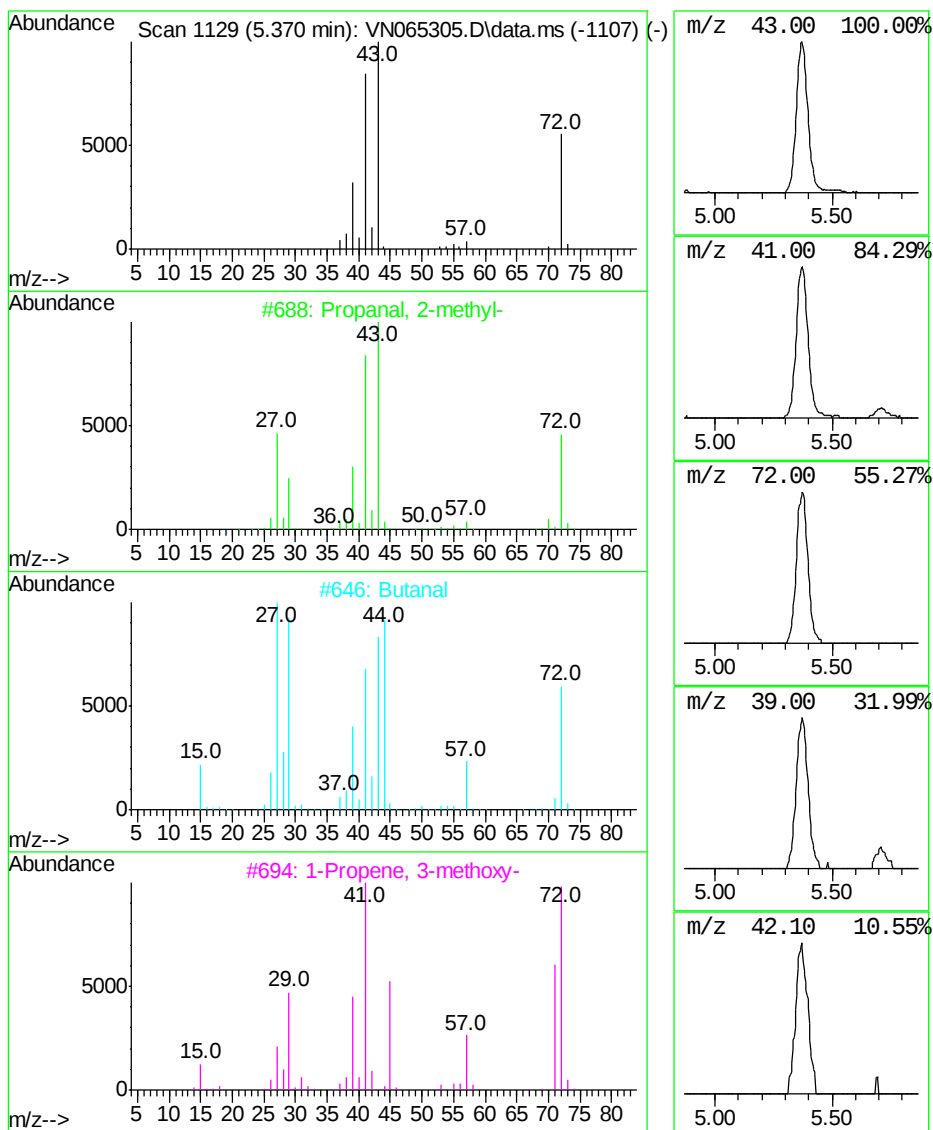
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanal, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.370	8.23 ug/l	142608	Pentafluorobenzene	7.627

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	Propanal, 2-methyl-	72	C4H8O	000078-84-2	91
2	Butanal	72	C4H8O	000123-72-8	58
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	53
4	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	33
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065305.D
Acq On : 29 Dec 2020 14:46
Operator : JC/MD
Sample : L5226-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
16882

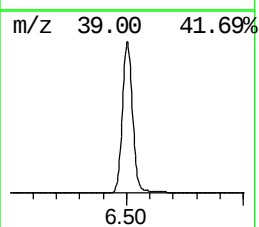
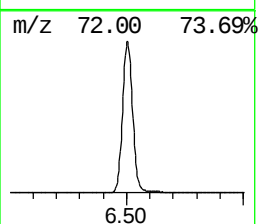
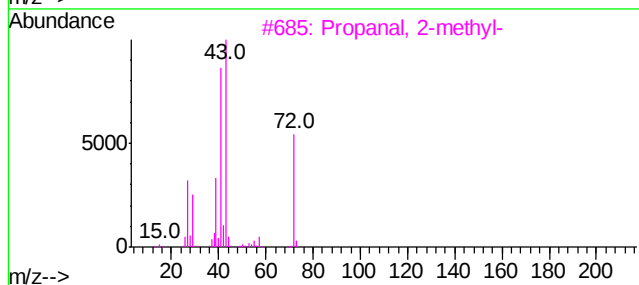
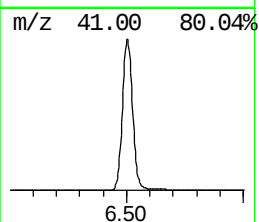
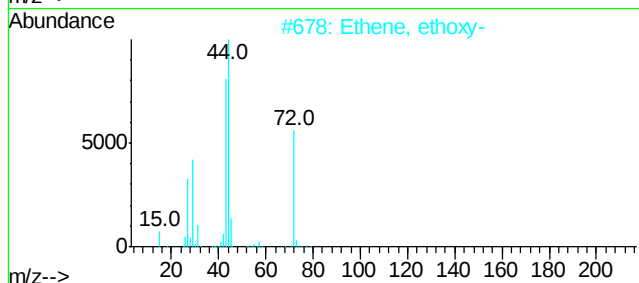
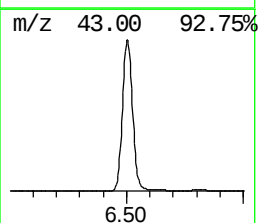
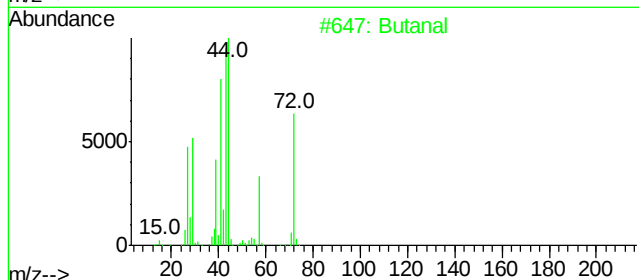
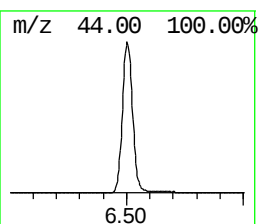
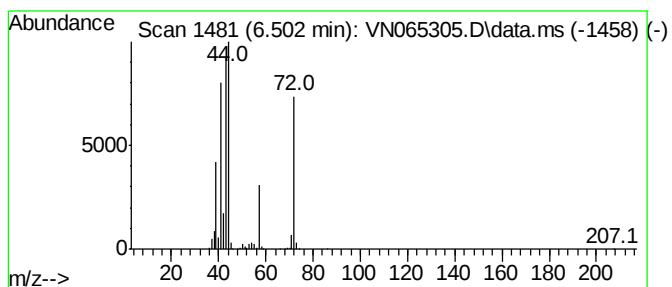
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.502	279.16 ug/l	4839700	Pentafluorobenzene	7.627

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	58
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	58
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	47
5	Isobutylene epoxide	72	C4H8O	000558-30-5	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065305.D
Acq On : 29 Dec 2020 14:46
Operator : JC/MD
Sample : L5226-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
16882

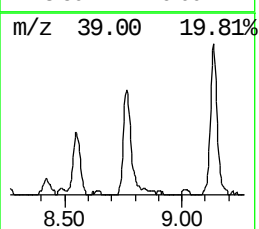
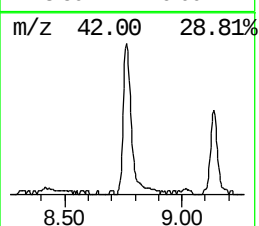
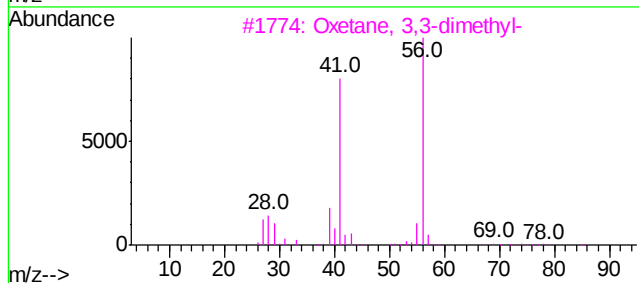
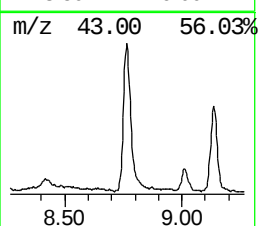
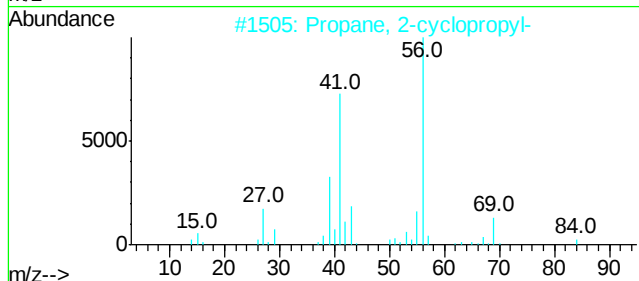
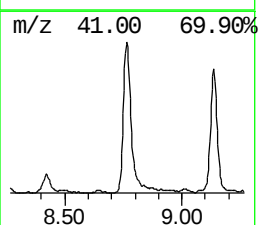
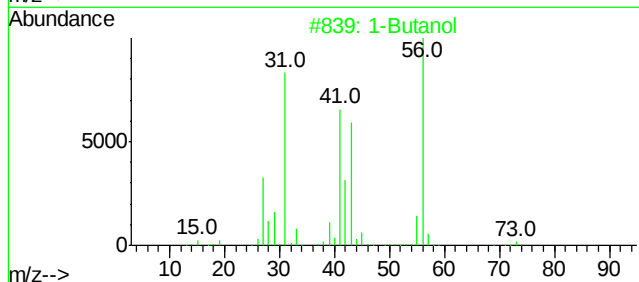
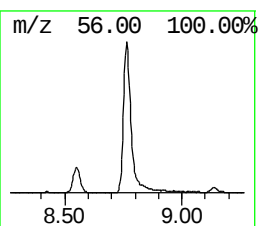
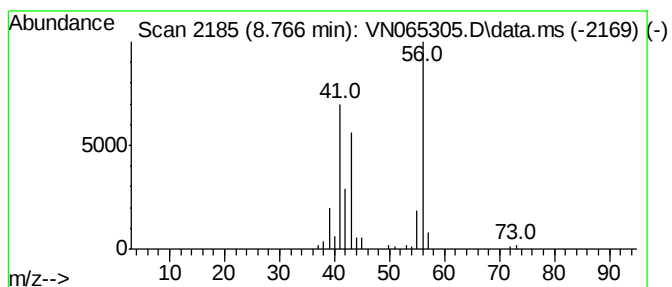
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.766	8.91 ug/l	184838	1,4-Difluorobenzene	8.550

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	83
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
3	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	36
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	9
5	Propane, 1-isocyano-	69	C4H7N	000627-36-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065305.D
Acq On : 29 Dec 2020 14:46
Operator : JC/MD
Sample : L5226-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
16882

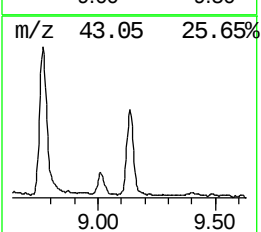
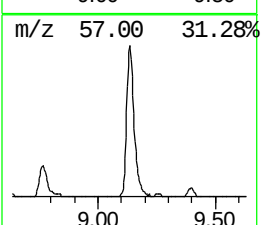
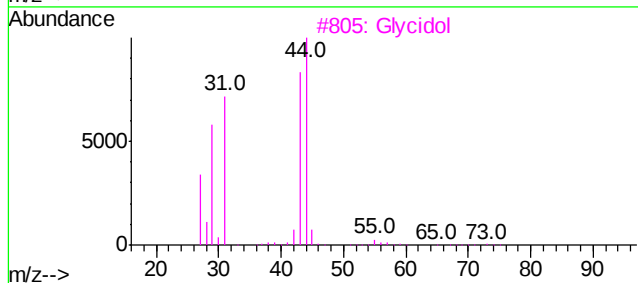
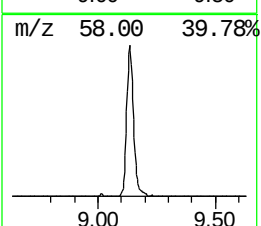
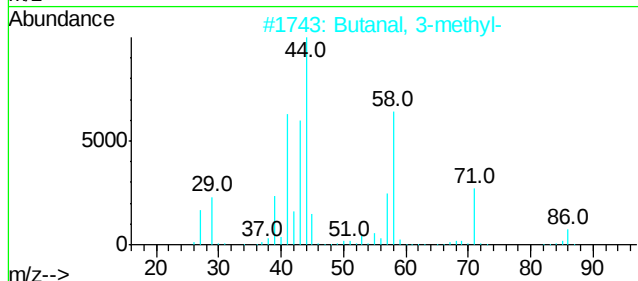
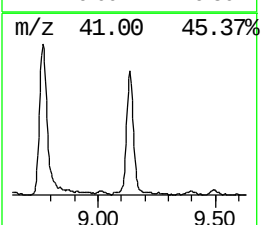
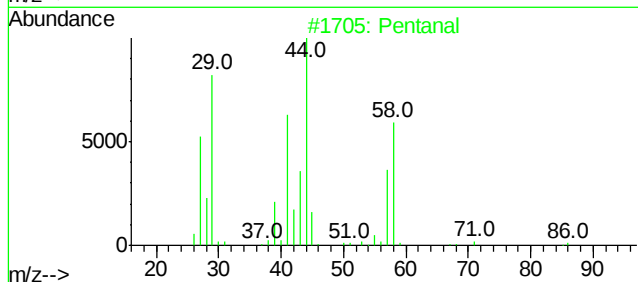
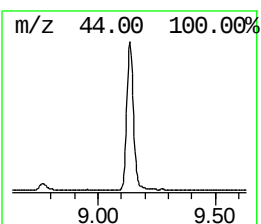
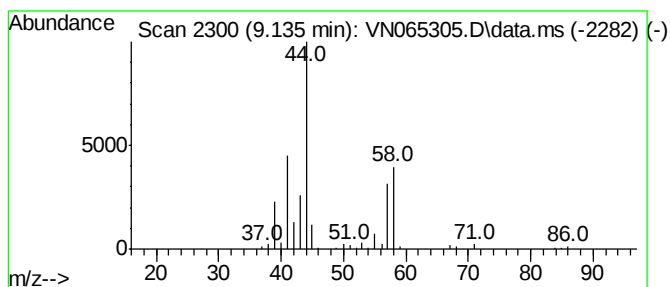
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.135	10.07 ug/l	208910	1,4-Difluorobenzene	8.550

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	91
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	74
3	Glycidol	74	C3H6O2	000556-52-5	33
4	Cyclopropyl carbinol	72	C4H8O	002516-33-8	28
5	Butane, 2-nitro-	103	C4H9NO2	000600-24-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065305.D
Acq On : 29 Dec 2020 14:46
Operator : JC/MD
Sample : L5226-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
16882

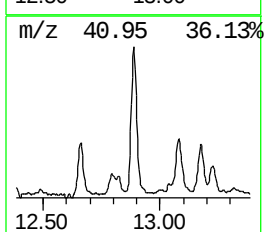
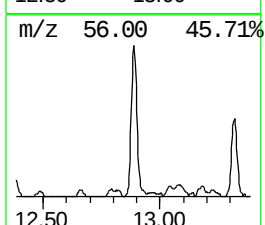
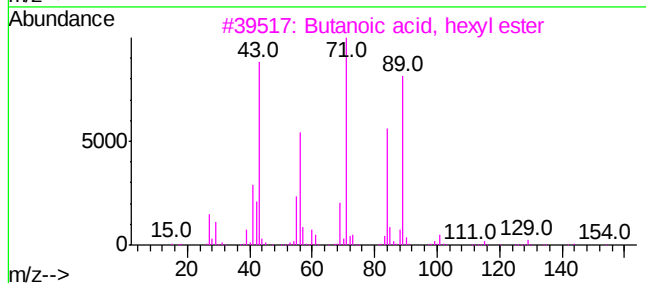
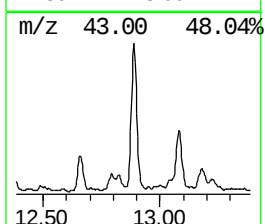
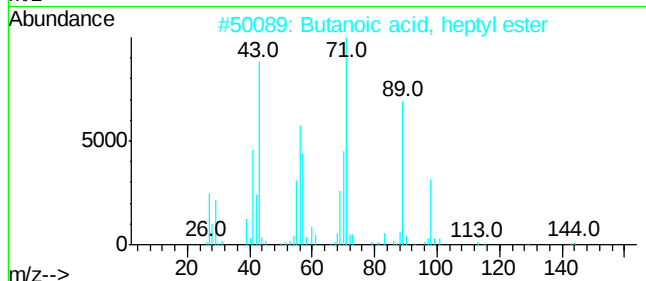
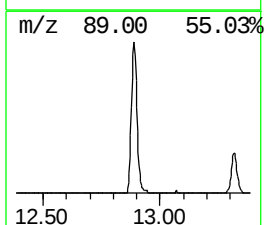
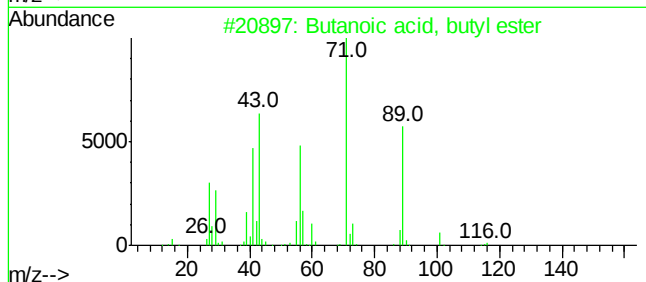
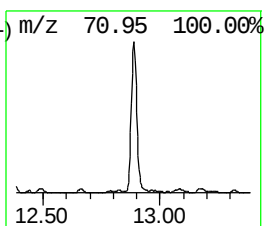
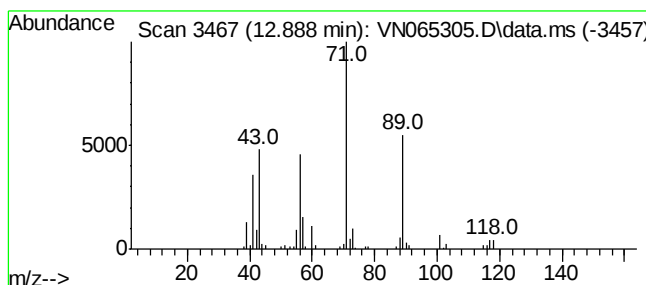
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Butanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.887	6.55 ug/l	134179	1,4-Dichlorobenzene-d4	13.318

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	64
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
4	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	64
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
 Data File : VN065305.D
 Acq On : 29 Dec 2020 14:46
 Operator : JC/MD
 Sample : L5226-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 16882

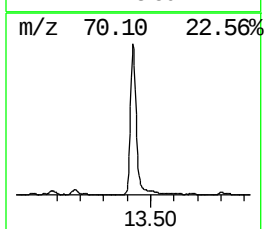
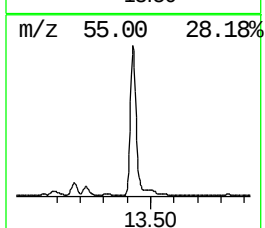
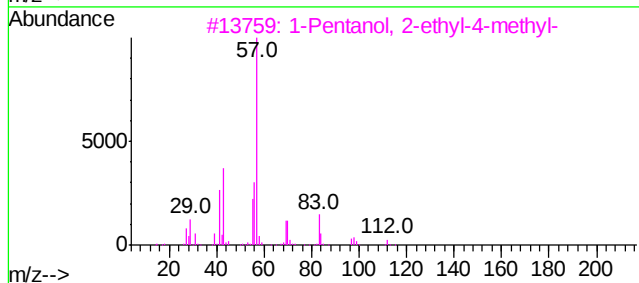
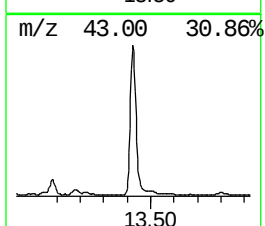
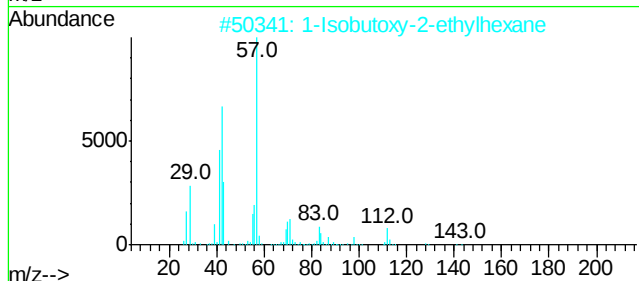
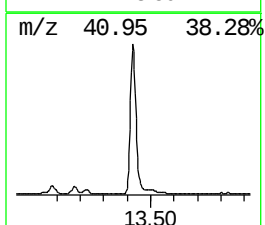
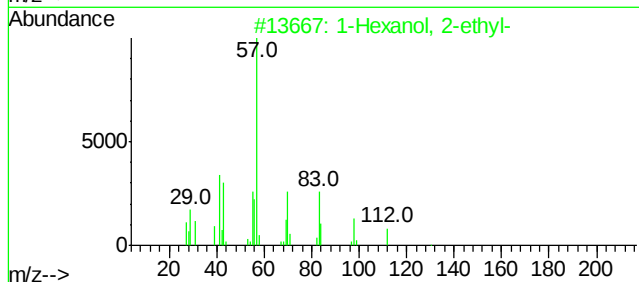
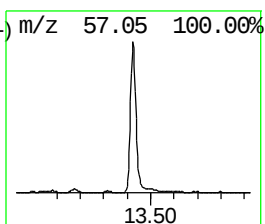
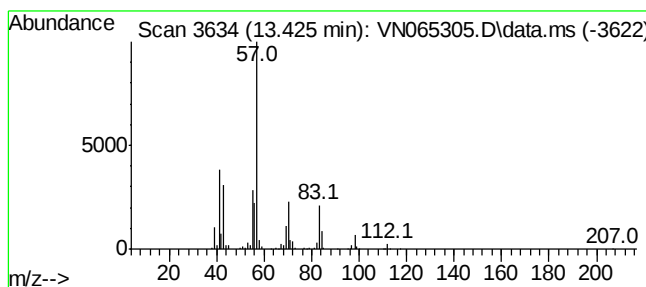
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
 Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.425	36.56 ug/l	748448	1,4-Dichlorobenzene-d4	13.318

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065305.D
Acq On : 29 Dec 2020 14:46
Operator : JC/MD
Sample : L5226-02
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
16882

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.296	151.9	ug/l	2633070	1	7.627	866829	50.0
Propanal, 2-met...	5.370	8.2	ug/l	142608	1	7.627	866829	50.0
Butanal	6.502	279.2	ug/l	4839700	1	7.627	866829	50.0
1-Butanol	8.766	8.9	ug/l	184838	2	8.550	1037260	50.0
Pentanal	9.135	10.1	ug/l	208910	2	8.550	1037260	50.0
Butanoic acid, ...	12.887	6.5	ug/l	134179	4	13.318	1023510	50.0
1-Hexanol, 2-et...	13.425	36.6	ug/l	748448	4	13.318	1023510	50.0