

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN122718\
 Data File : VN053208.D
 Acq On : 27 Dec 2018 13:16
 Operator : MD\SY
 Sample : J6571-03 10X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 30061

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\82N121818W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.989	57	67	79	rBV	382838	517691	1.55%	0.411%
2	2.317	157	169	188	rBV	590913	965785	2.88%	0.767%
3	3.696	579	598	623	rBV	11067742	27927193	83.38%	22.183%
4	3.815	625	635	671	rVB2	193759	565095	1.69%	0.449%
5	4.259	753	773	823	rVB	917456	2790545	8.33%	2.217%
6	6.027	1299	1323	1371	rBV	1585789	4960655	14.81%	3.940%
7	7.593	1790	1810	1821	rBV	654038	1649090	4.92%	1.310%
8	7.667	1821	1833	1856	rVB	1332130	3125201	9.33%	2.482%
9	8.027	1926	1945	1967	rBV	706901	1637212	4.89%	1.300%
10	8.586	2102	2119	2166	rVB	2297388	4748155	14.18%	3.771%
11	8.840	2185	2198	2210	rBV	213368	411824	1.23%	0.327%
12	10.091	2571	2587	2604	rBV	3147547	5698502	17.01%	4.526%
13	10.348	2651	2667	2698	rVV	19413480	33493304	100.00%	26.604%
14	10.493	2698	2712	2745	rVB	12614761	21109630	63.03%	16.767%
15	10.805	2787	2809	2845	rBV	909583	2727576	8.14%	2.167%
16	11.406	2977	2996	3017	rBV	2984423	5230440	15.62%	4.155%
17	12.400	3284	3305	3327	rBV	2315564	4036377	12.05%	3.206%
18	13.342	3587	3598	3621	rVB	2614343	4302267	12.85%	3.417%

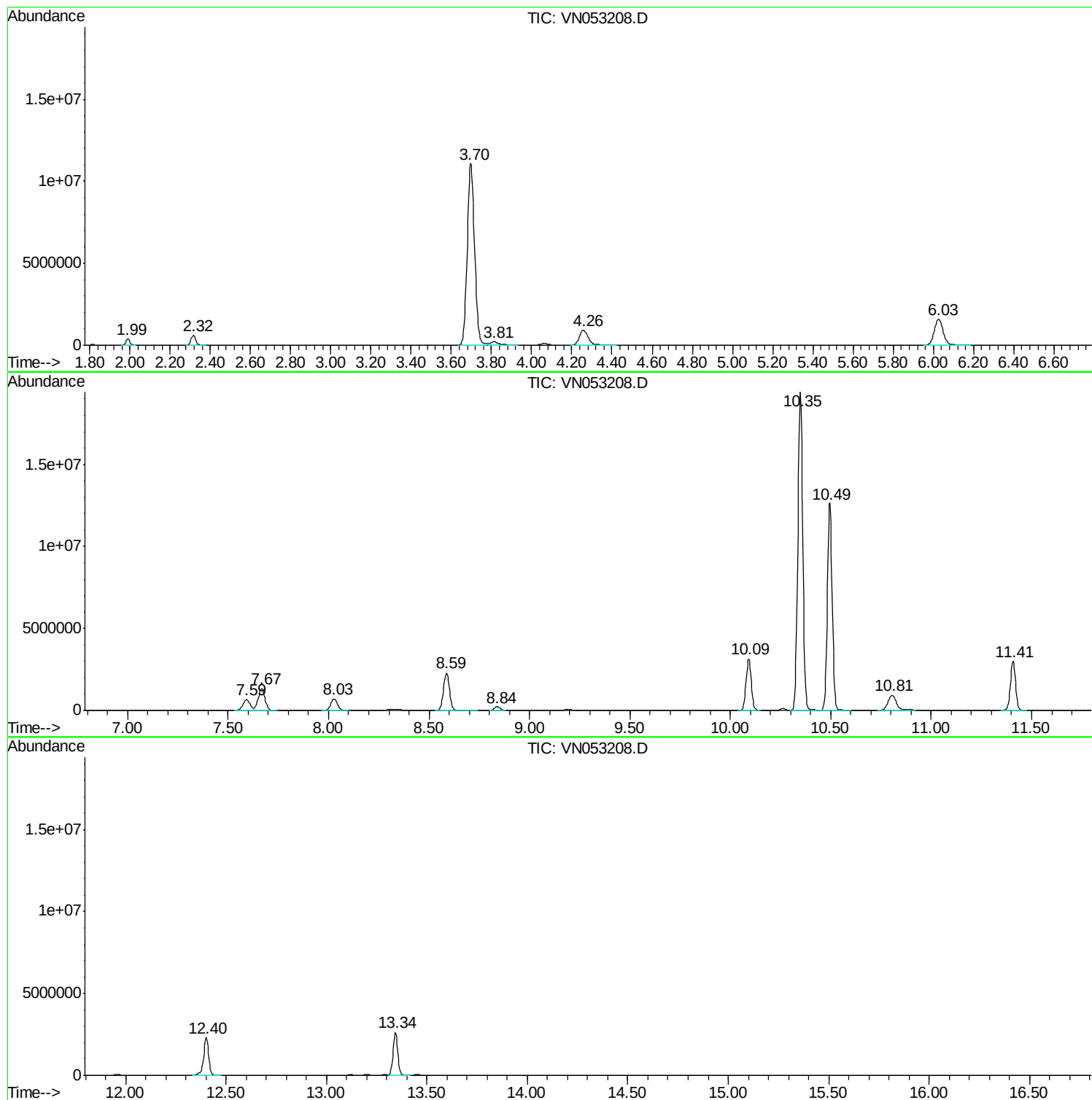
Sum of corrected areas: 125896542

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN122718\
Data File : VN053208.D
Acq On : 27 Dec 2018 13:16
Operator : MD\SY
Sample : J6571-03 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
30061

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN122718\
Data File : VN053208.D
Acq On : 27 Dec 2018 13:16
Operator : MD\SY
Sample : J6571-03 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
30061

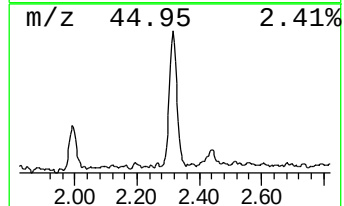
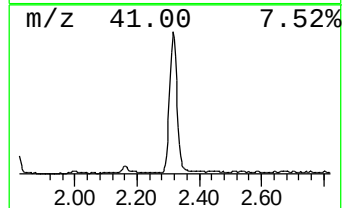
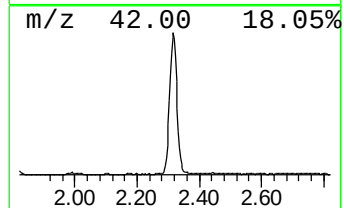
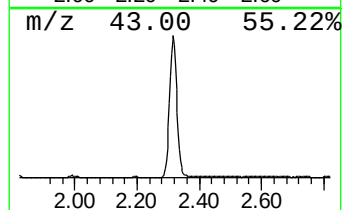
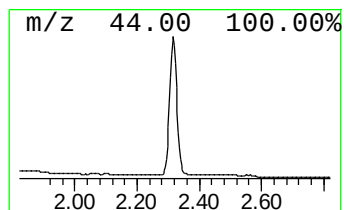
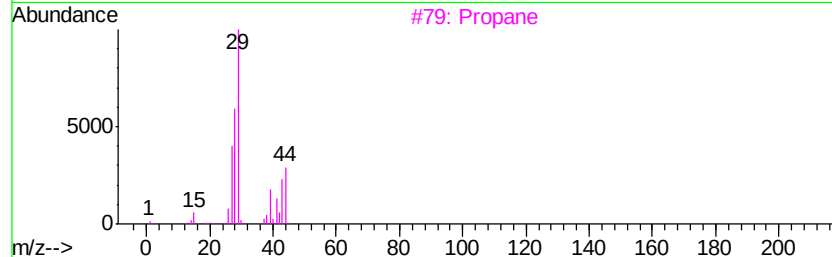
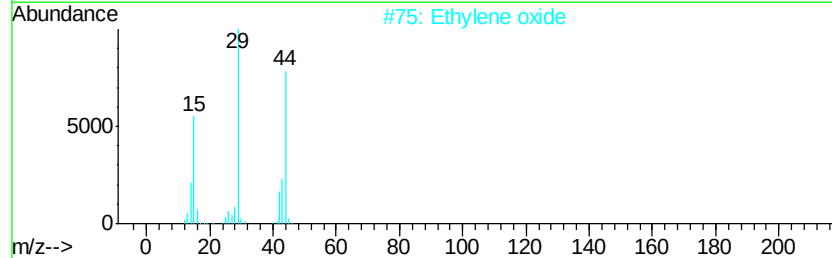
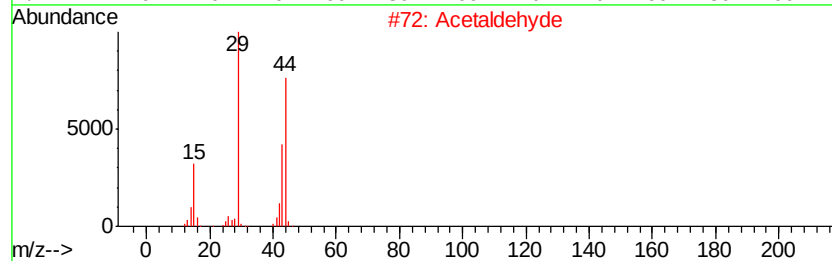
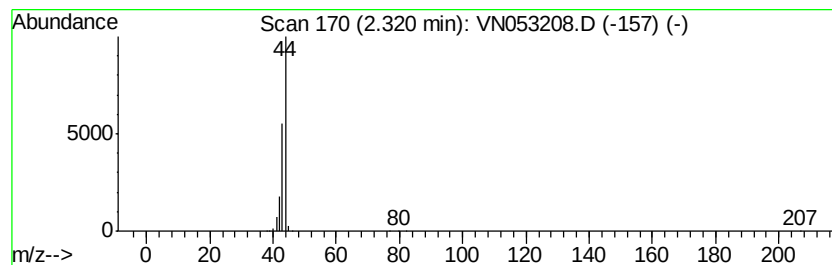
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	15.45 ug/l	965785	Pentafluorobenzene	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetaldehyde	44	C2H4O	000075-07-0	64
2		Ethylene oxide	44	C2H4O	000075-21-8	5
3		Propane	44	C3H8	000074-98-6	4
4		Alanine	89	C3H7NO2	000056-41-7	4
5		Carbon dioxide	44	CO2	000124-38-9	3



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN122718\
Data File : VN053208.D
Acq On : 27 Dec 2018 13:16
Operator : MD\SY
Sample : J6571-03 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 28

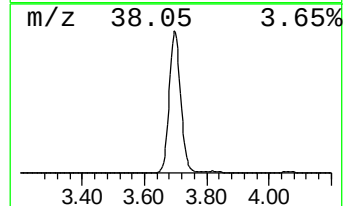
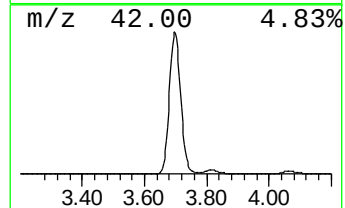
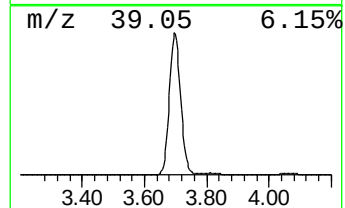
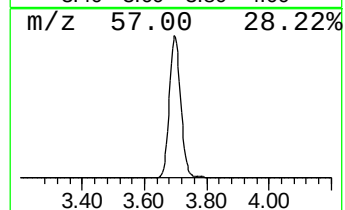
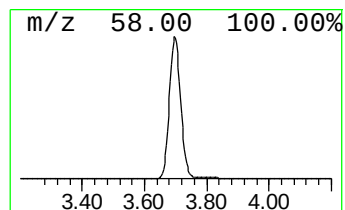
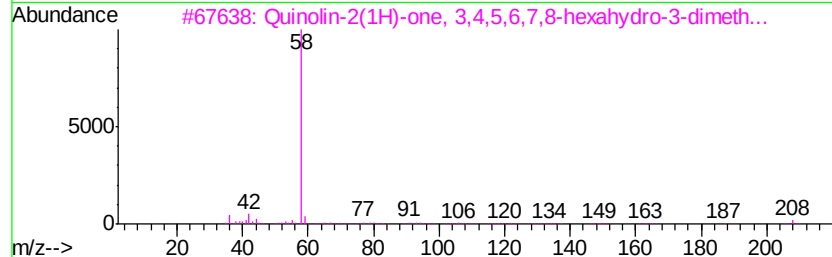
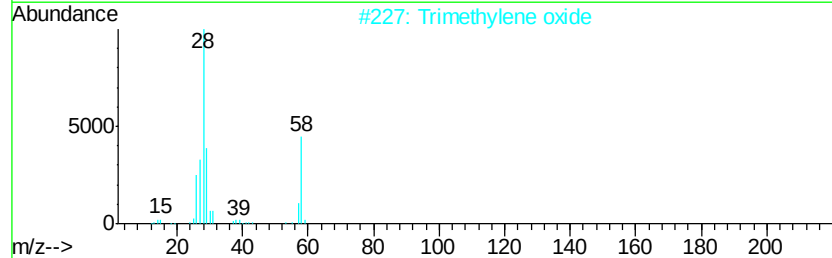
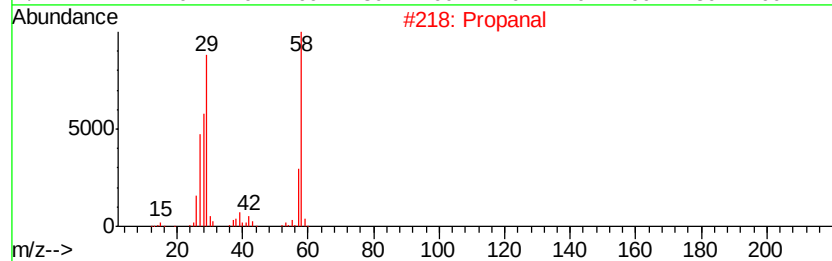
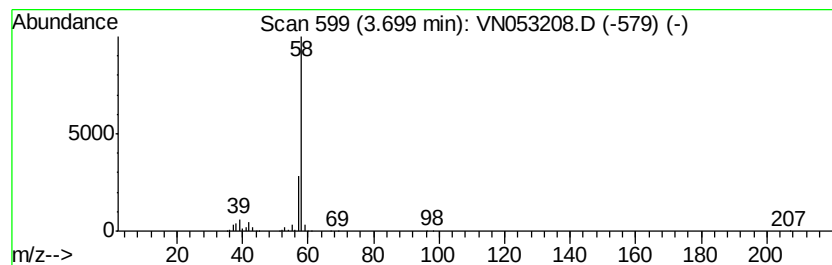
Instrument :
MSVOA_N
ClientSampleId :
30061

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
3.70	446.81 ug/l	27927200	Pentafluorobenzene	7.67		
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	64
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...		208	C12H20N2O	1000259-95-6	9
4	Propylene oxide		58	C3H6O	000075-56-9	7
5	Oxirane, methyl-, (S)-		58	C3H6O	016088-62-3	4



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN122718\
Data File : VN053208.D
Acq On : 27 Dec 2018 13:16
Operator : MD\SY
Sample : J6571-03 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
30061

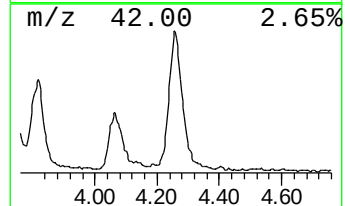
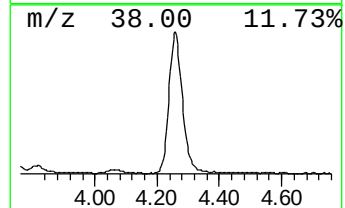
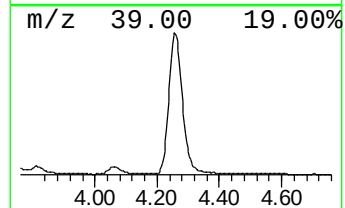
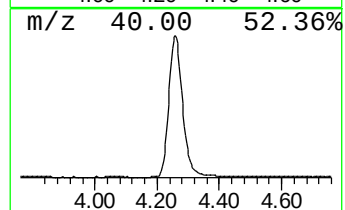
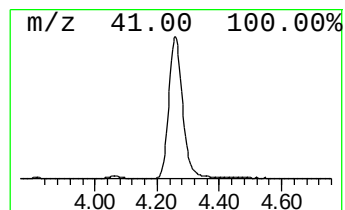
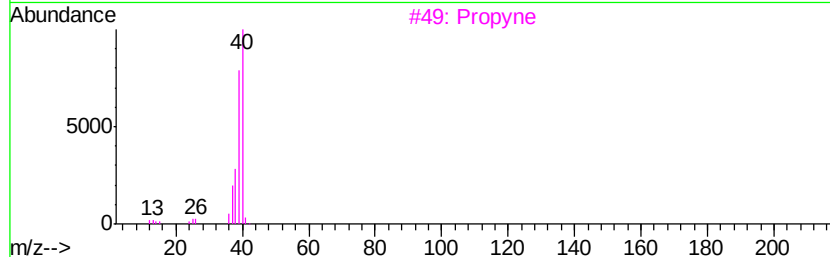
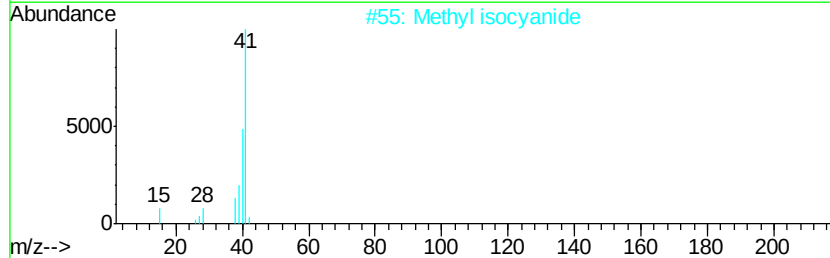
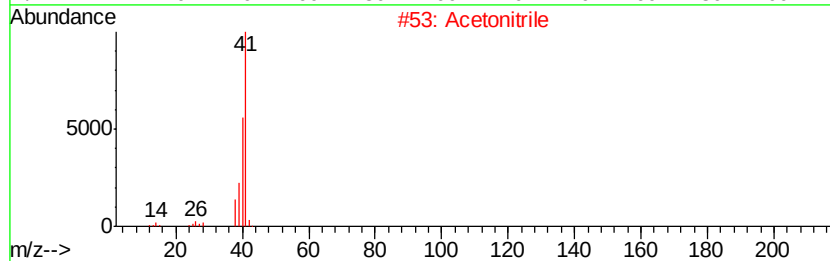
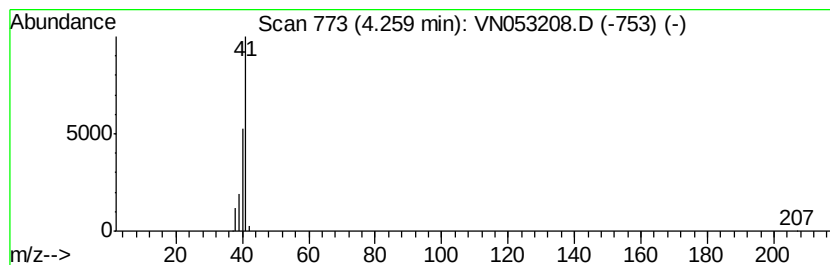
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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

Peak Number 4 Acetonitrile Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.26	44.65 ug/l	2790550	Pentafluorobenzene	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetonitrile	41	C2H3N	000075-05-8	64
2		Methyl isocyanide	41	C2H3N	000593-75-9	64
3		Propyne	40	C3H4	000074-99-7	4
4		Allene	40	C3H4	000463-49-0	1
5		Oxalic acid, diallyl ester	170	C8H10O4	1000309-22-9	1



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN122718\
Data File : VN053208.D
Acq On : 27 Dec 2018 13:16
Operator : MD\SY
Sample : J6571-03 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
30061

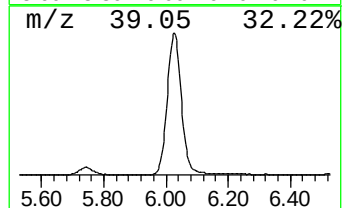
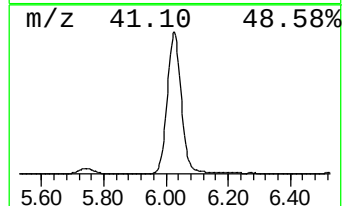
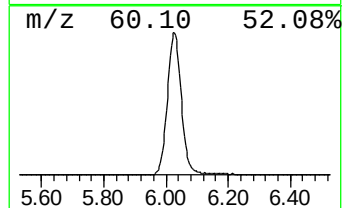
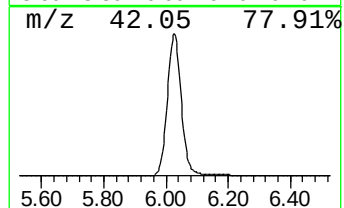
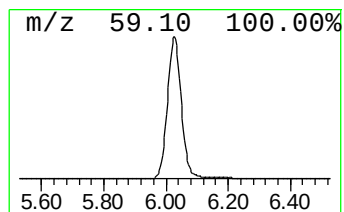
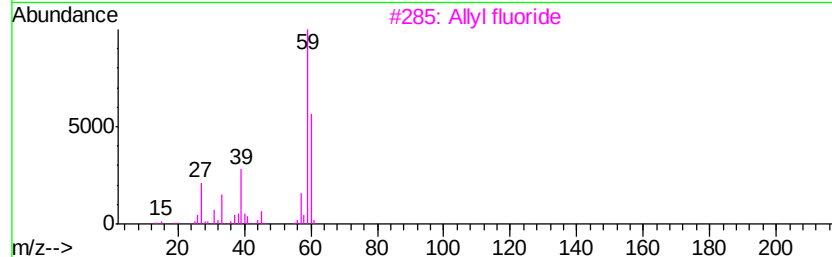
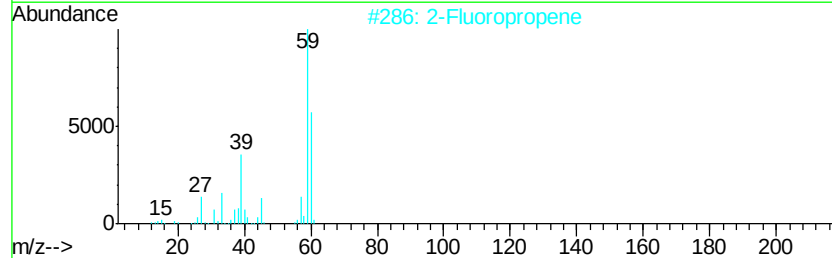
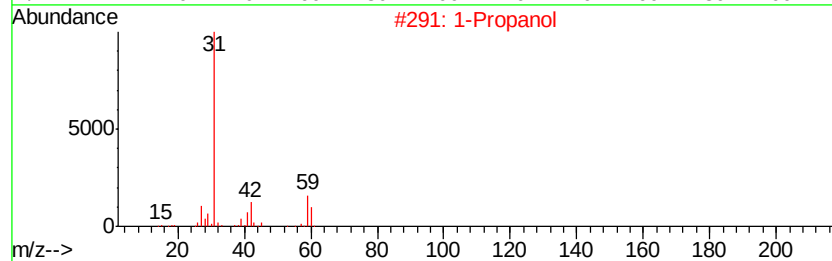
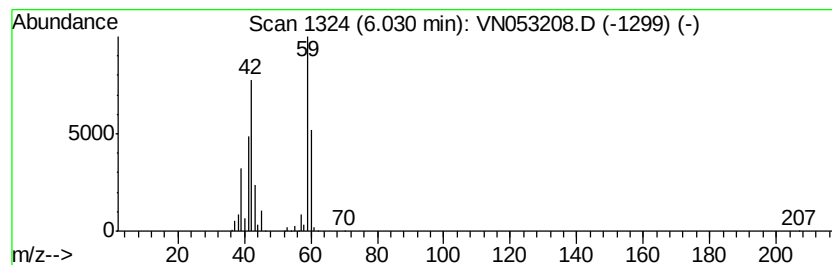
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.03	79.37 ug/l	4960660	Pentafluorobenzene	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	78
2		2-Fluoropropene	60	C3H5F	001184-60-7	38
3		Allyl fluoride	60	C3H5F	000818-92-8	37
4		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	25
5		2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	17



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN122718\
Data File : VN053208.D
Acq On : 27 Dec 2018 13:16
Operator : MD\SY
Sample : J6571-03 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 28

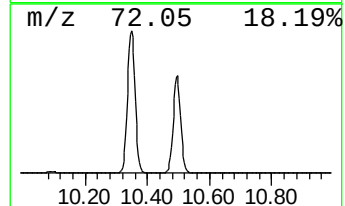
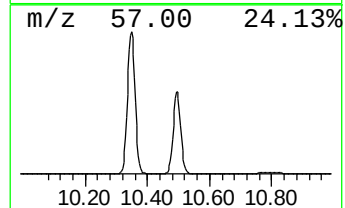
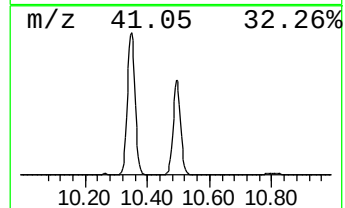
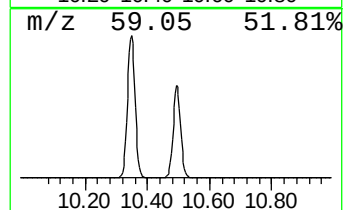
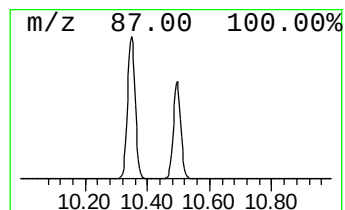
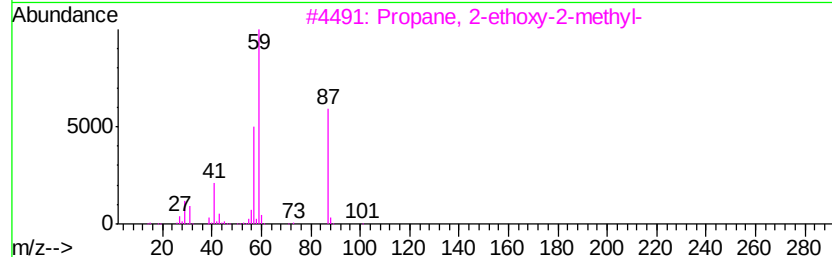
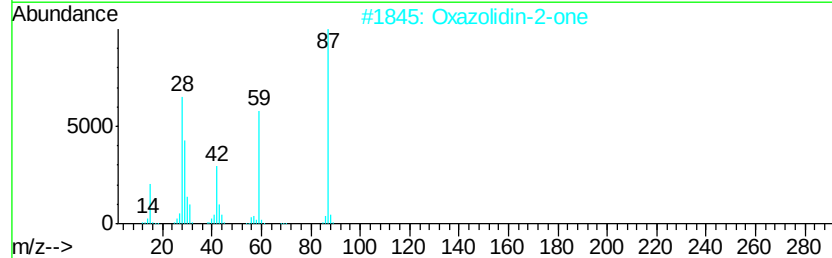
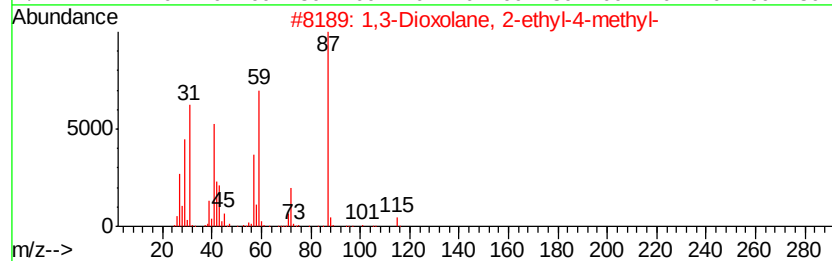
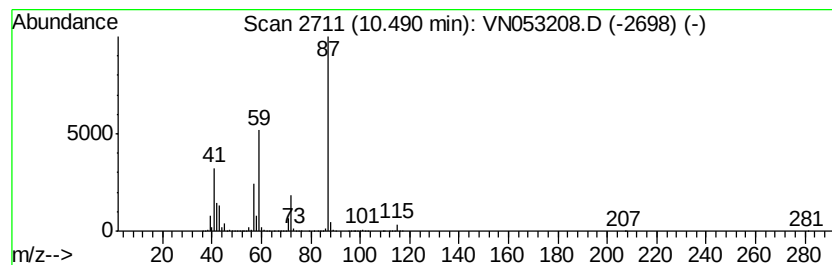
Instrument :
MSVOA_N
ClientSampleId :
30061

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.49	201.80 ug/l	21109600	Chlorobenzene-d5	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	80
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	64
4	2-Propanone, 0-methyloxime	87	C4H9NO	003376-35-0	52
5	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN122718\
Data File : VN053208.D
Acq On : 27 Dec 2018 13:16
Operator : MD\SY
Sample : J6571-03 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
30061

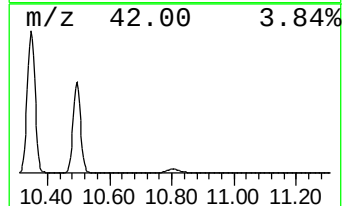
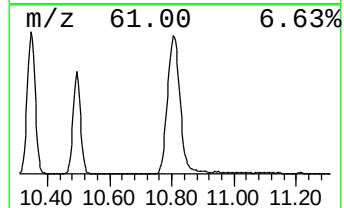
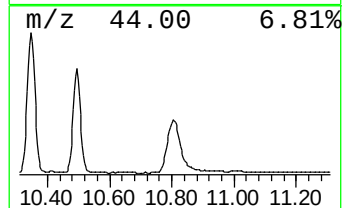
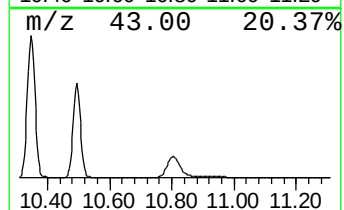
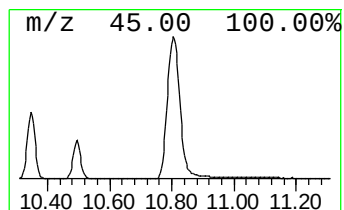
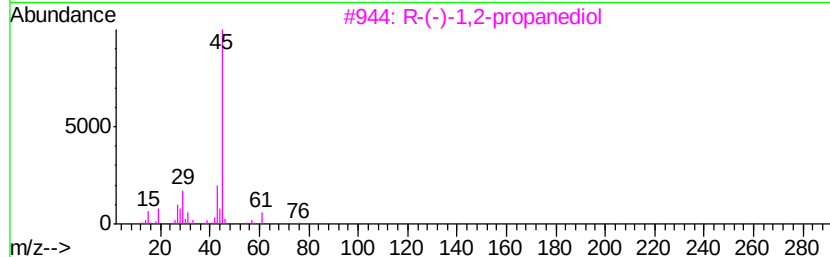
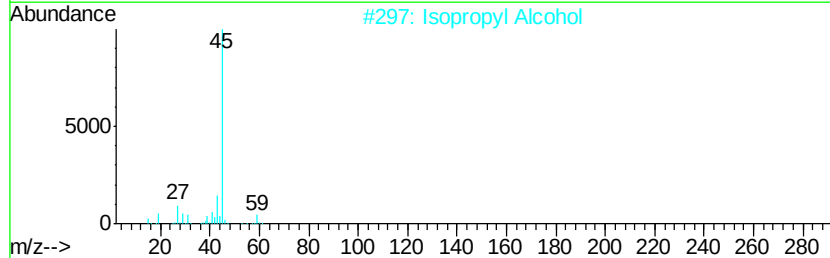
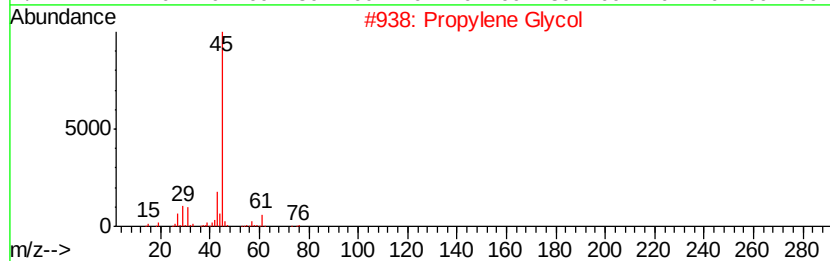
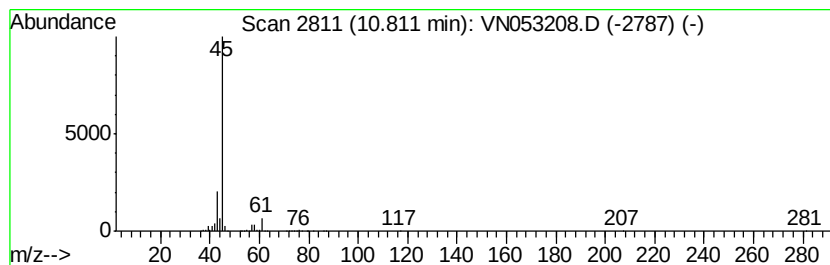
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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

Peak Number 8 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	26.07 ug/l	2727580	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90	
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	80	
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78	
4	2-Pentanol	88	C5H12O	006032-29-7	9	
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9	



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN122718\
Data File : VN053208.D
Acq On : 27 Dec 2018 13:16
Operator : MD\SY
Sample : J6571-03 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
30061

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.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	2.32	15.4	ug/l	965785	1	7.67	3125200	50.0
Propanal	3.70	446.8	ug/l	27927200	1	7.67	3125200	50.0
Acetonitrile	4.26	44.6	ug/l	2790550	1	7.67	3125200	50.0
1-Propanol	6.03	79.4	ug/l	4960660	1	7.67	3125200	50.0
1,3-Dioxolane, 2-...	10.49	201.8	ug/l	21109600	3	11.41	5230440	50.0
Propylene Glycol	10.81	26.1	ug/l	2727580	3	11.41	5230440	50.0