

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061021\
 Data File : VX022653.D
 Acq On : 10 Jun 2021 19:16
 Operator : JC/MD
 Sample : M2645-03 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BUR-1041

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_X\Method\82X061021W.M

Title : SW846 8260

Signal : TIC: VX022653.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	71	rBV	400842	438563	38.00%	11.018%
2	2.075	155	162	175	rBV	770888	1154135	100.00%	28.994%
3	2.239	185	189	195	rVV	11876	18699	1.62%	0.470%
4	2.294	195	198	208	rVB	7234	13165	1.14%	0.331%
5	2.386	208	213	221	rVB	12086	20418	1.77%	0.513%
6	3.337	362	369	376	rBV2	6047	13027	1.13%	0.327%
7	3.867	449	456	466	rVB3	10025	25375	2.20%	0.637%
8	4.574	563	572	583	rBV3	7673	23886	2.07%	0.600%
9	5.391	696	706	719	rBV2	40328	118809	10.29%	2.985%
10	5.556	723	733	744	rBV	69241	195489	16.94%	4.911%
11	5.970	790	801	813	rBV2	52564	142777	12.37%	3.587%
12	6.367	856	866	876	rBV2	9724	25271	2.19%	0.635%
13	6.769	922	932	947	rBV2	123523	290853	25.20%	7.307%
14	8.555	1219	1225	1234	rBV2	11929	21033	1.82%	0.528%
15	8.653	1234	1241	1248	rBV	259264	400177	34.67%	10.053%
16	10.055	1465	1471	1487	rBV	248194	343022	29.72%	8.617%
17	11.085	1634	1640	1652	rVB	191531	241877	20.96%	6.076%
18	12.024	1789	1794	1802	rBV	246028	300467	26.03%	7.548%
19	12.585	1880	1886	1898	rBV5	8238	15181	1.32%	0.381%
20	13.103	1968	1971	1985	rVB2	9037	16044	1.39%	0.403%
21	13.426	2018	2024	2036	rBV	71898	122525	10.62%	3.078%
22	13.890	2097	2100	2110	rVB5	7448	11853	1.03%	0.298%
23	14.195	2145	2150	2157	rBV2	17107	27907	2.42%	0.701%

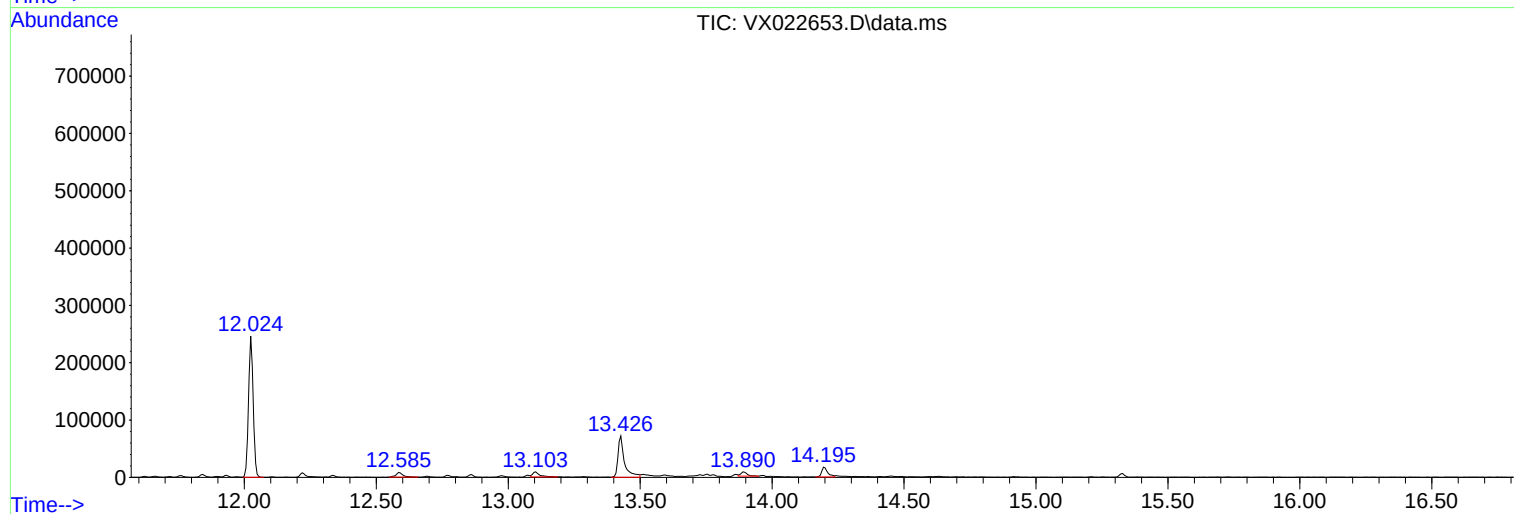
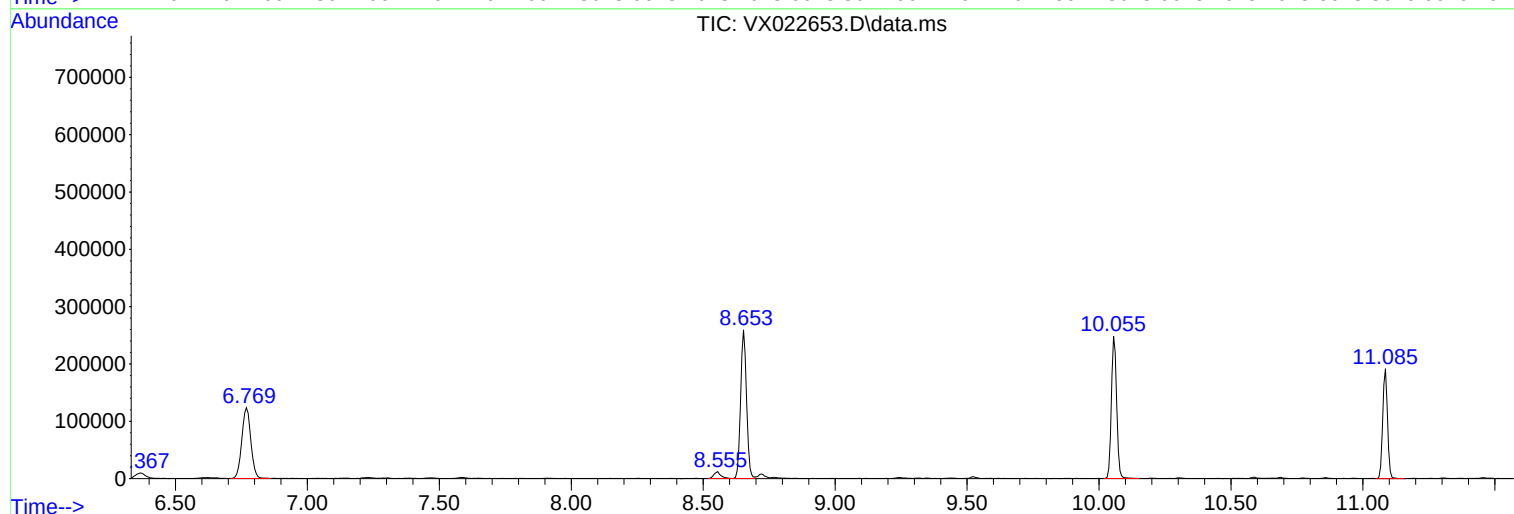
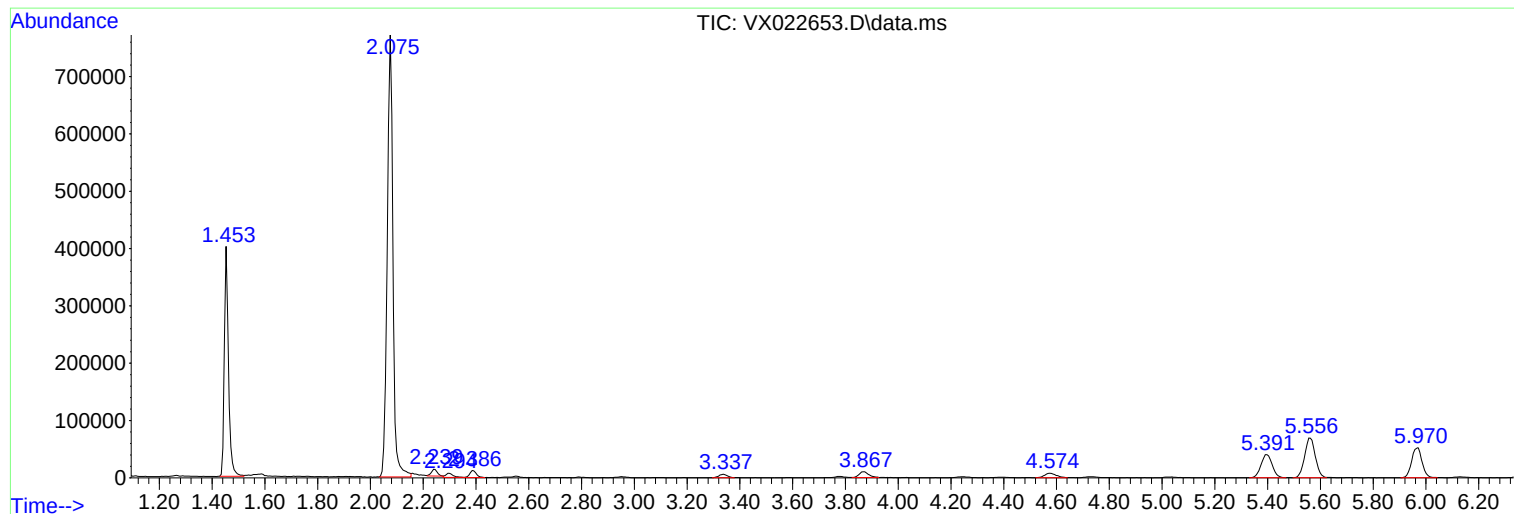
Sum of corrected areas: 3980553

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061021\
Data File : VX022653.D
Acq On : 10 Jun 2021 19:16
Operator : JC/MD
Sample : M2645-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1041

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061021\
Data File : VX022653.D
Acq On : 10 Jun 2021 19:16
Operator : JC/MD
Sample : M2645-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1041

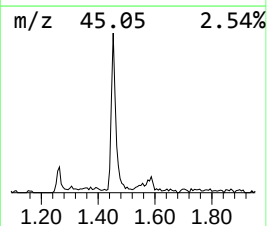
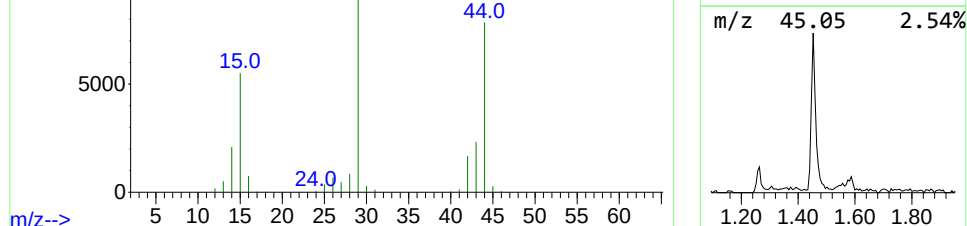
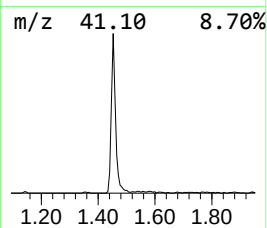
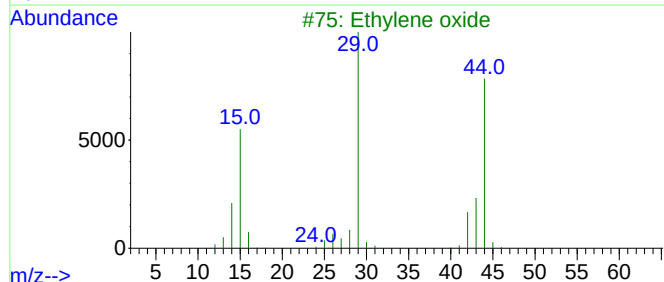
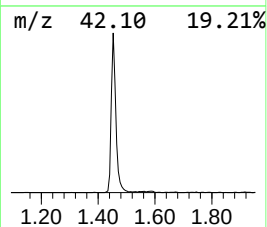
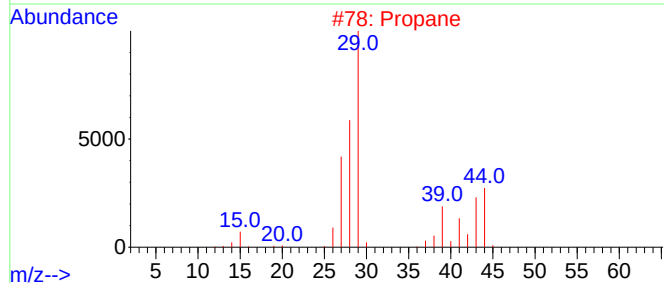
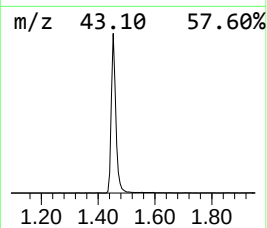
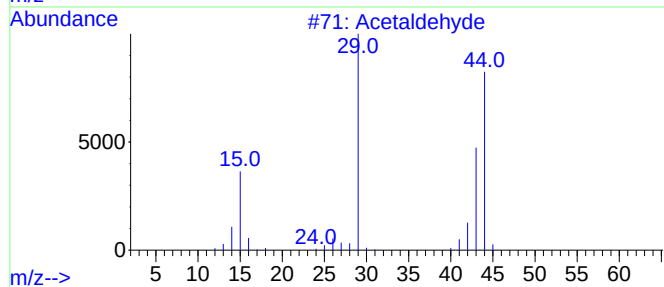
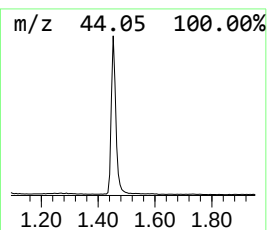
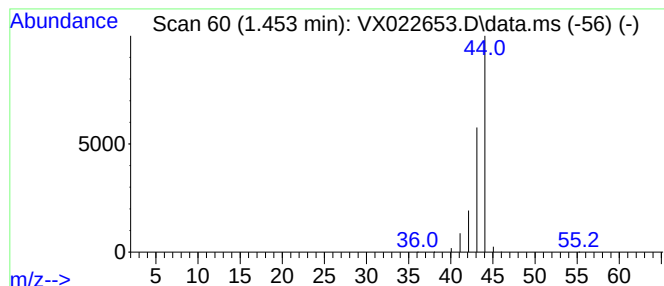
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	112.17 ug/l	438563	Pentafluorobenzene	5.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetaldehyde	44	C2H4O	000075-07-0	9
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		Carbon dioxide	44	CO2	000124-38-9	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061021\
Data File : VX022653.D
Acq On : 10 Jun 2021 19:16
Operator : JC/MD
Sample : M2645-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1041

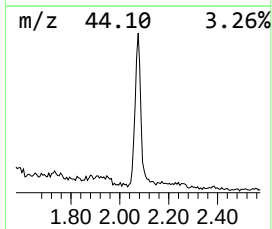
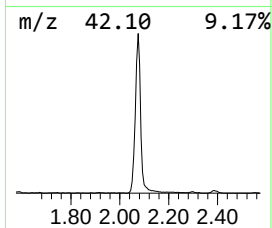
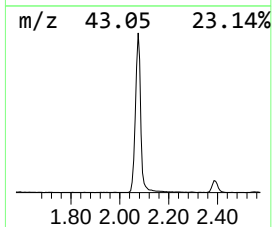
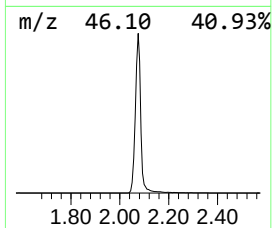
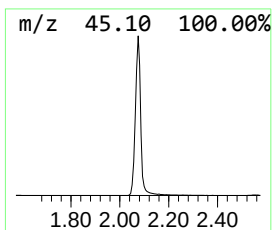
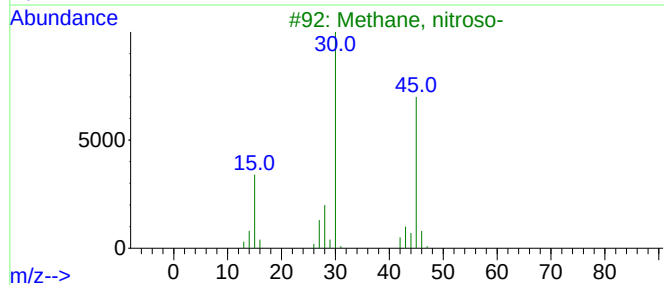
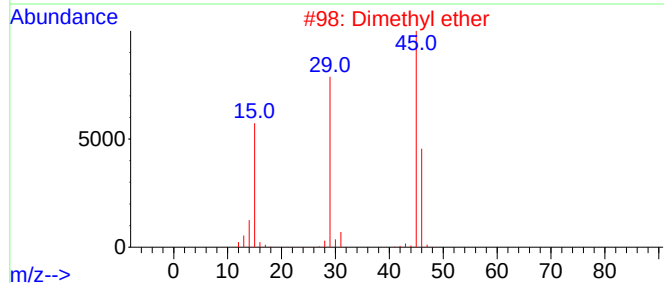
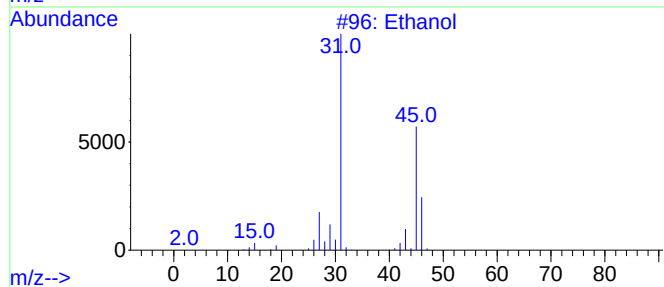
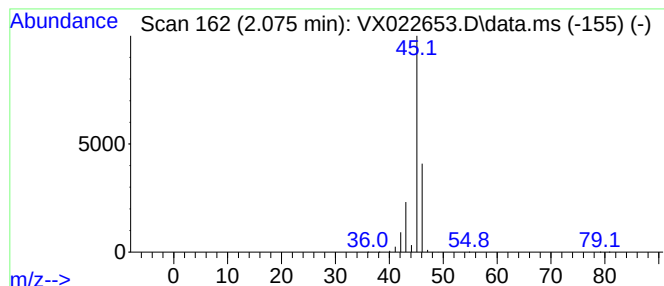
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.075	295.19 ug/l	1154140	Pentafluorobenzene	5.562

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	9
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_X\Data\VX061021\
Data File : VX022653.D
Acq On : 10 Jun 2021 19:16
Operator : JC/MD
Sample : M2645-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1041

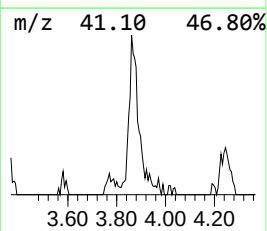
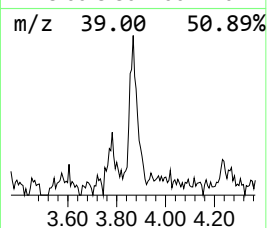
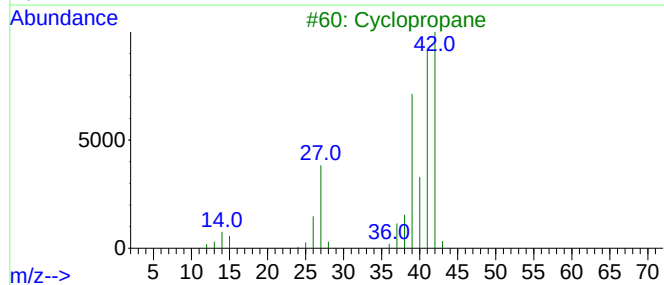
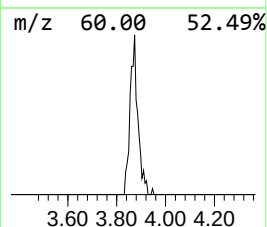
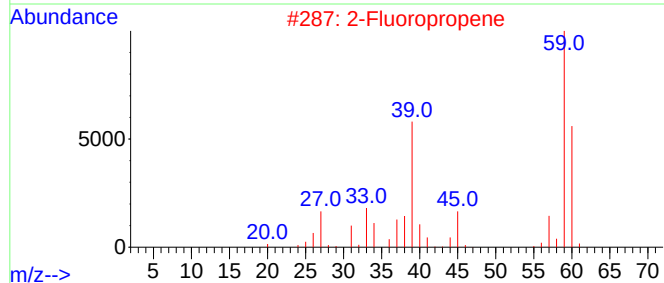
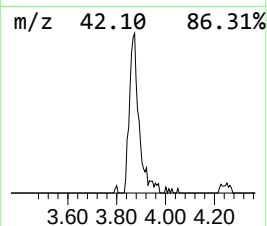
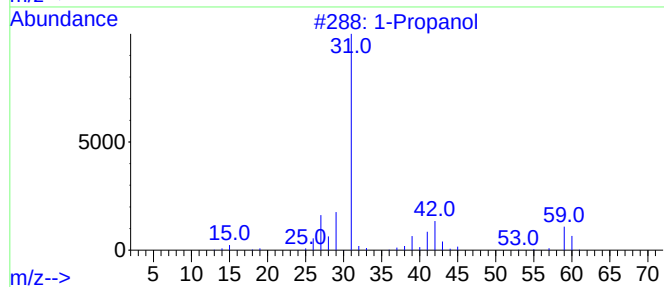
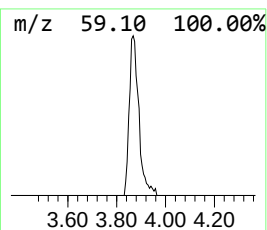
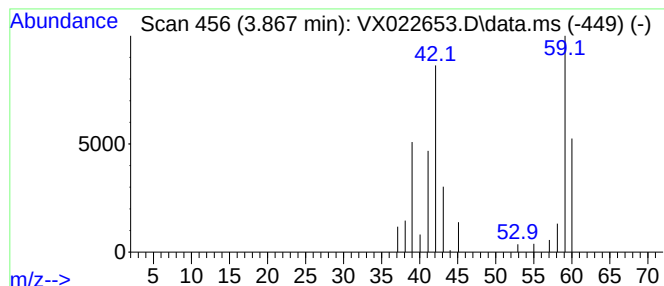
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.867	6.49 ug/l	25375	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	50
2	2-Fluoropropene			60	C3H5F	001184-60-7	43
3	Cyclopropane			42	C3H6	000075-19-4	9
4	Methylenecyclopropane			54	C4H6	006142-73-0	9
5	Acetaldoxime			59	C2H5NO	000107-29-9	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061021\
Data File : VX022653.D
Acq On : 10 Jun 2021 19:16
Operator : JC/MD
Sample : M2645-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

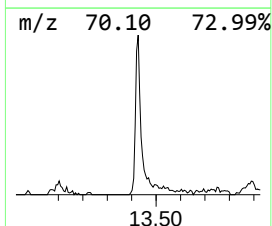
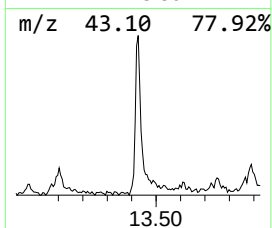
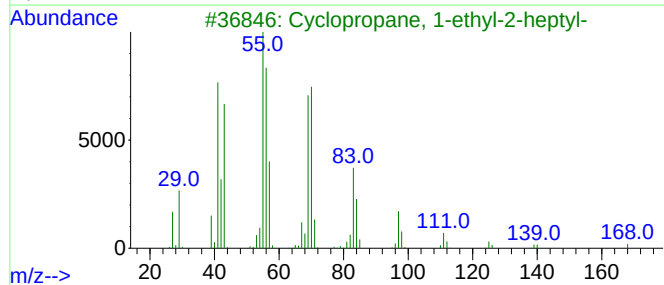
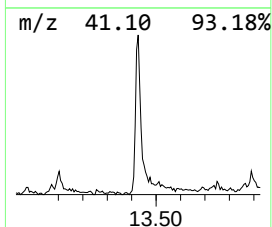
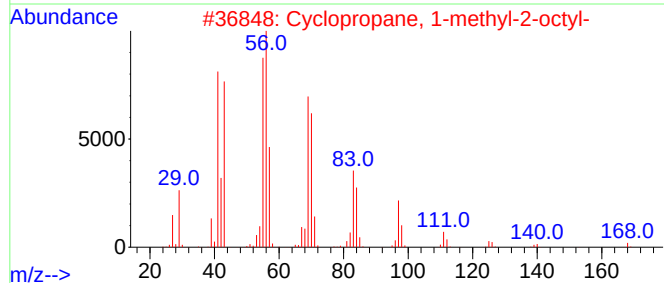
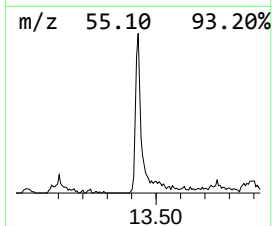
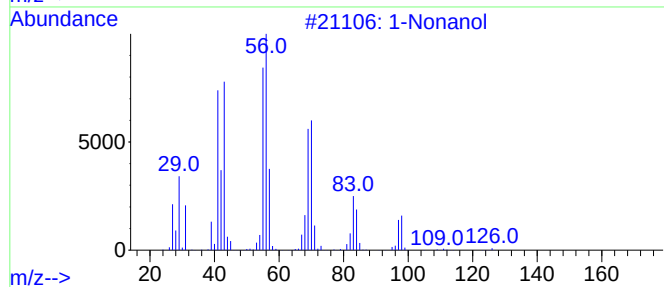
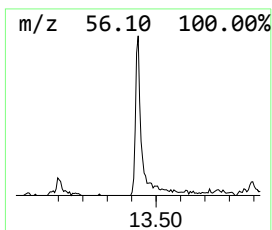
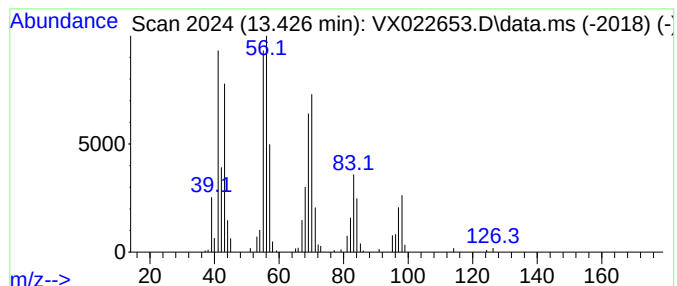
Instrument :
MSVOA_X
ClientSampleId :
BUR-1041

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Nonanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.426	20.39 ug/l	122525	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	86
2	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	80
3	Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	80
4	Cycloheptane	98	C7H14	000291-64-5	64
5	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061021\
Data File : VX022653.D
Acq On : 10 Jun 2021 19:16
Operator : JC/MD
Sample : M2645-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1041

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.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
unknown-01	1.453	112.2	ug/l	438563	1	5.562	195489	50.0
Ethanol	2.075	295.2	ug/l	1154140	1	5.562	195489	50.0
1-Propanol	3.867	6.5	ug/l	25375	1	5.562	195489	50.0
1-Nonanol	13.426	20.4	ug/l	122525	4	12.024	300467	50.0