

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
 Data File : VX020757.D
 Acq On : 26 Jan 2021 16:41
 Operator : JC/SP
 Sample : M1189-18
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 41107

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\82X012521W.M
 Title : SW846 8260

Signal : TIC: VX020757.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.160	9	12	21	rVB	268216	231308	11.69%	1.587%
2	1.374	44	47	54	rBV2	19382	28723	1.45%	0.197%
3	1.471	59	63	75	rVV	1109793	1275499	64.47%	8.753%
4	2.331	199	204	214	rVB	42733	73246	3.70%	0.503%
5	2.416	214	218	223	rBV	34551	53977	2.73%	0.370%
6	3.014	305	316	325	rVB2	8339	21434	1.08%	0.147%
7	3.386	367	377	384	rBV3	9411	21693	1.10%	0.149%
8	4.300	516	527	542	rBV	162764	443870	22.43%	3.046%
9	5.464	706	718	731	rBV2	226911	649013	32.80%	4.454%
10	5.623	734	744	759	rVB2	380961	1072862	54.22%	7.362%
11	6.031	800	811	819	rBV	246682	644807	32.59%	4.425%
12	6.111	819	824	832	rVB2	37302	95774	4.84%	0.657%
13	6.830	928	942	956	rBV	603796	1417812	71.66%	9.730%
14	7.019	965	973	982	rVB3	9449	24022	1.21%	0.165%
15	7.269	1002	1014	1023	rBV	34089	80462	4.07%	0.552%
16	7.629	1067	1073	1081	rBV	21139	40457	2.04%	0.278%
17	8.696	1240	1248	1255	rBV	1285505	1978550	100.00%	13.578%
18	8.763	1255	1259	1265	rVB	95047	142737	7.21%	0.980%
19	9.561	1387	1390	1397	rVB	14688	21066	1.06%	0.145%
20	10.092	1469	1477	1489	rBV	1300975	1753149	88.61%	12.031%
21	10.189	1489	1493	1497	rVV	20691	30605	1.55%	0.210%
22	10.232	1497	1500	1505	rVB	17189	23336	1.18%	0.160%
23	10.342	1509	1518	1524	rBV	72162	104551	5.28%	0.717%
24	10.683	1569	1574	1585	rVB	36124	61048	3.09%	0.419%
25	10.787	1585	1591	1601	rBV5	12941	23754	1.20%	0.163%
26	11.122	1640	1646	1651	rBV	1041521	1339958	67.72%	9.195%
27	11.171	1651	1654	1660	rVB	46606	57555	2.91%	0.395%
28	11.317	1674	1678	1687	rBV7	12361	20218	1.02%	0.139%
29	11.457	1696	1701	1704	rVB2	20501	29449	1.49%	0.202%
30	11.610	1721	1726	1729	rBV2	16745	21997	1.11%	0.151%
31	11.719	1738	1744	1751	rBV	182832	213992	10.82%	1.469%
32	11.793	1751	1756	1760	rVB	26231	32210	1.63%	0.221%
33	11.902	1770	1774	1782	rBV	46406	69672	3.52%	0.478%
34	12.024	1790	1794	1796	rBV	157151	189890	9.60%	1.303%
35	12.061	1796	1800	1807	rVB	1385713	1682176	85.02%	11.544%
36	12.256	1827	1832	1841	rBV	141047	231428	11.70%	1.588%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020757.D
Acq On : 26 Jan 2021 16:41
Operator : JC/SP
Sample : M1189-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41107

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\82X012521W.M
Title : SW846 8260

37	12.347	1842	1847	1853	rVB5	18749	39104	1.98%	0.268%
38	12.823	1918	1925	1932	rBV8	18553	33340	1.69%	0.229%
39	13.646	2054	2060	2068	rBV	29529	42147	2.13%	0.289%
40	13.817	2084	2088	2093	rVB	48028	62249	3.15%	0.427%
41	13.884	2094	2099	2106	rVV	26295	40200	2.03%	0.276%
42	13.951	2106	2110	2126	rVB	28369	46225	2.34%	0.317%
43	14.073	2126	2130	2134	rBV2	18301	21465	1.08%	0.147%
44	14.676	2227	2229	2236	rVB	15928	19955	1.01%	0.137%
45	14.792	2242	2248	2251	rBV	34720	43705	2.21%	0.300%
46	15.536	2364	2370	2375	rBV4	14441	21395	1.08%	0.147%

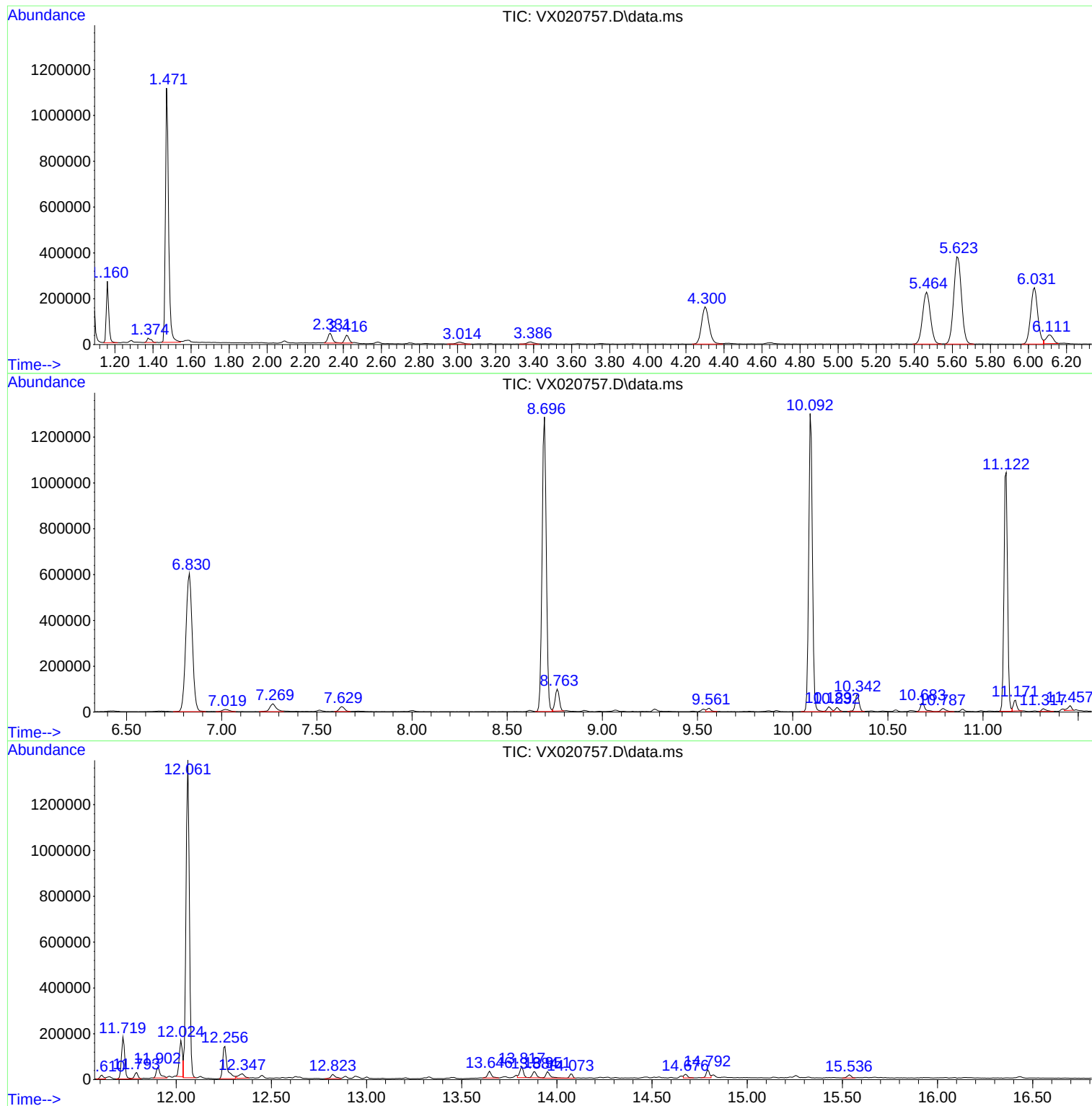
Sum of corrected areas: 14572085

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020757.D
Acq On : 26 Jan 2021 16:41
Operator : JC/SP
Sample : M1189-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41107

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020757.D
Acq On : 26 Jan 2021 16:41
Operator : JC/SP
Sample : M1189-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41107

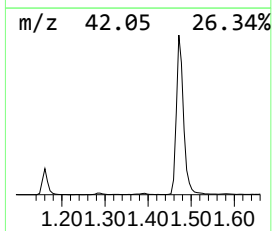
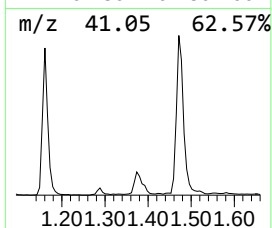
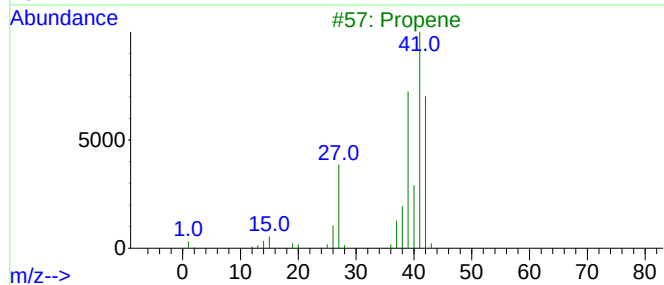
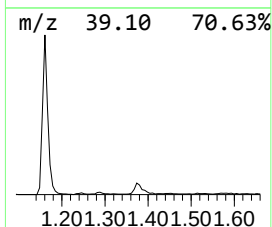
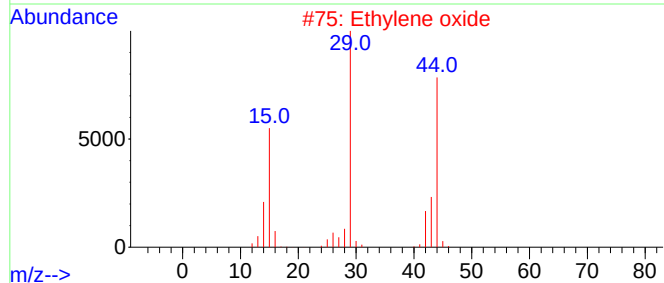
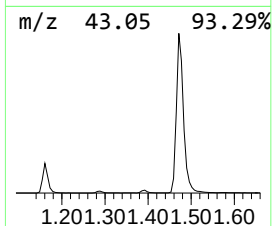
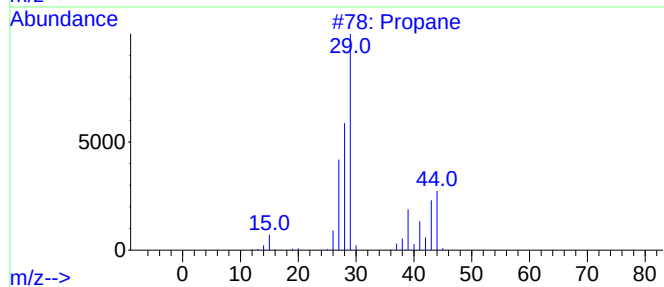
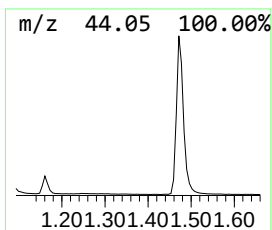
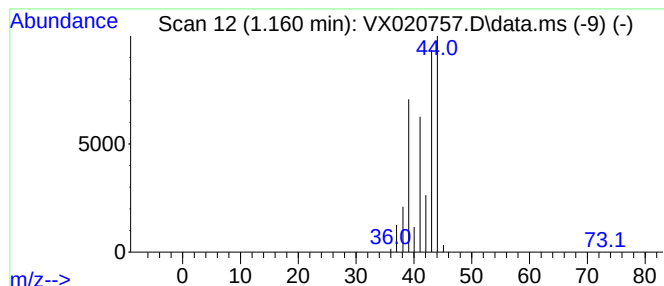
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.160	10.78 ug/l	231308	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	90
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propene	42	C3H6	000115-07-1	4
4			Acetaldehyde	44	C2H4O	000075-07-0	3
5			Ethyne, fluoro-	44	C2HF	002713-09-9	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020757.D
Acq On : 26 Jan 2021 16:41
Operator : JC/SP
Sample : M1189-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41107

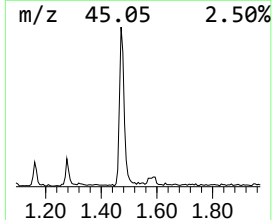
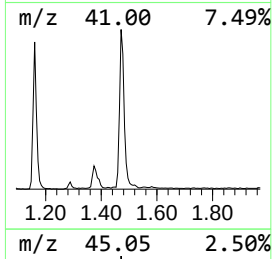
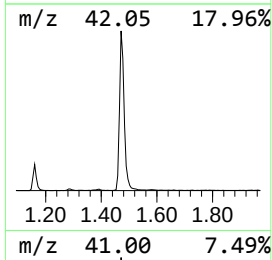
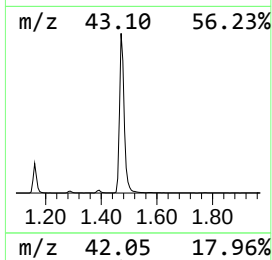
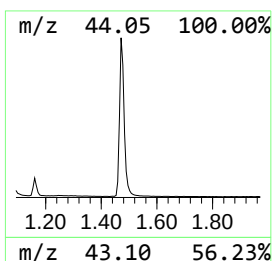
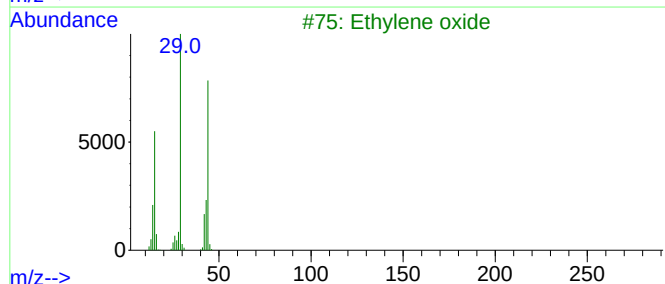
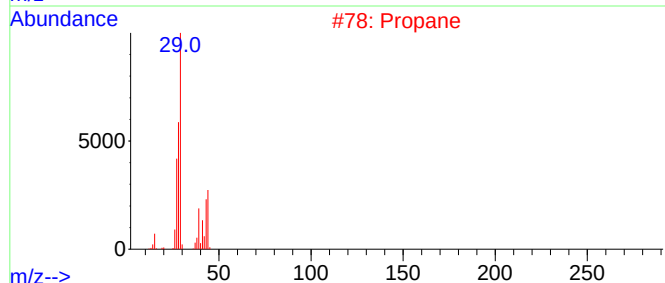
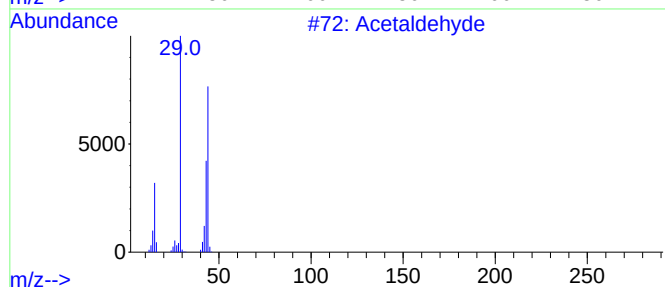
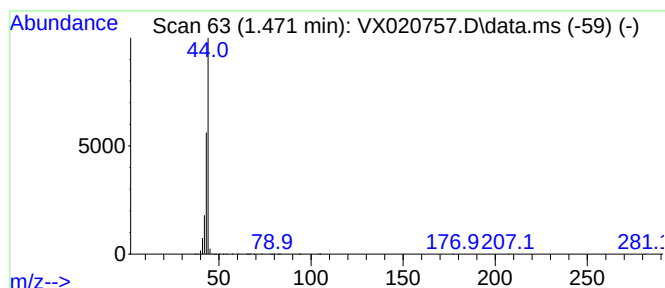
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.471	59.44 ug/l	1275500	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
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\VX012621\
Data File : VX020757.D
Acq On : 26 Jan 2021 16:41
Operator : JC/SP
Sample : M1189-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41107

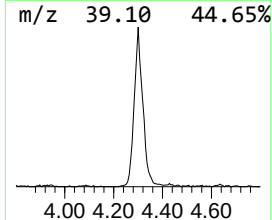
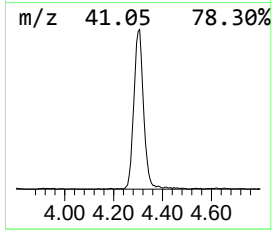
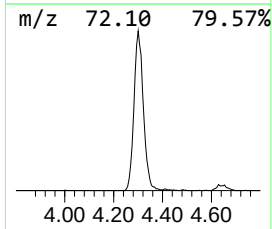
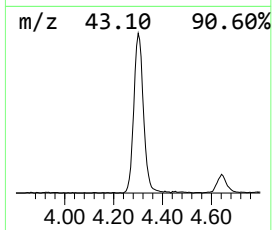
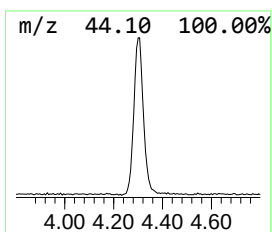
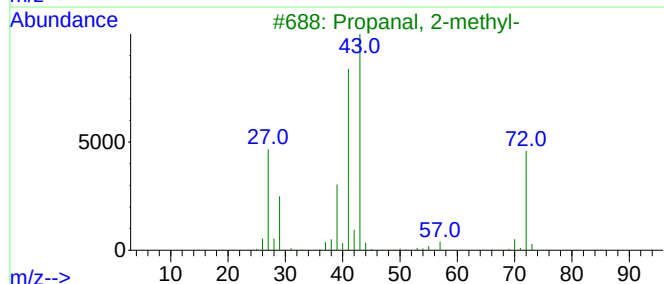
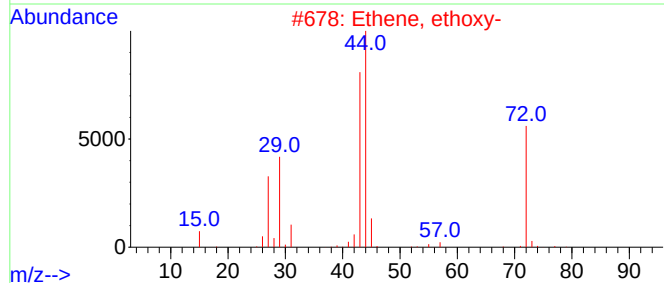
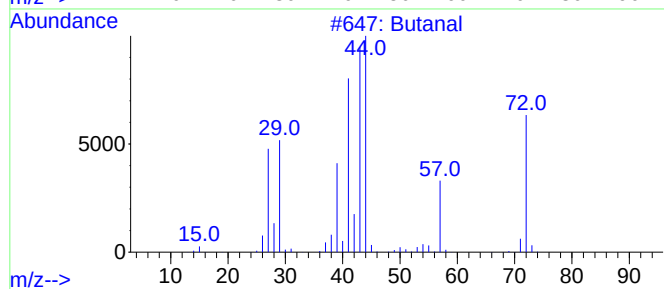
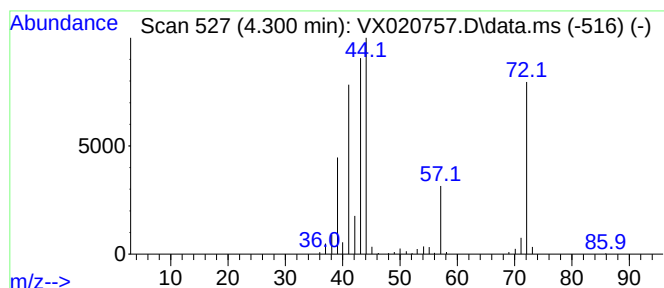
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.300	20.69 ug/l	443870	Pentafluorobenzene	5.629

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	53
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
5			Isobutylene epoxide	72	C4H8O	000558-30-5	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020757.D
Acq On : 26 Jan 2021 16:41
Operator : JC/SP
Sample : M1189-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41107

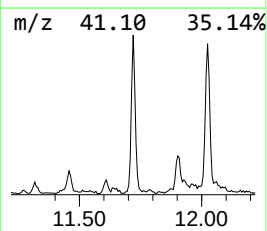
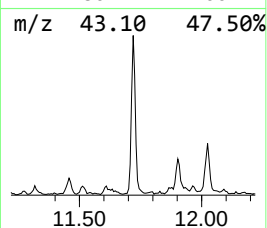
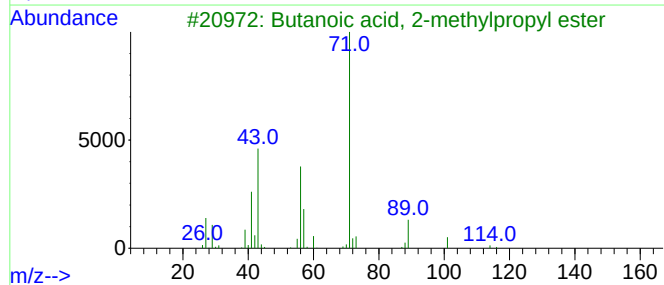
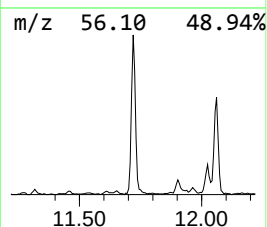
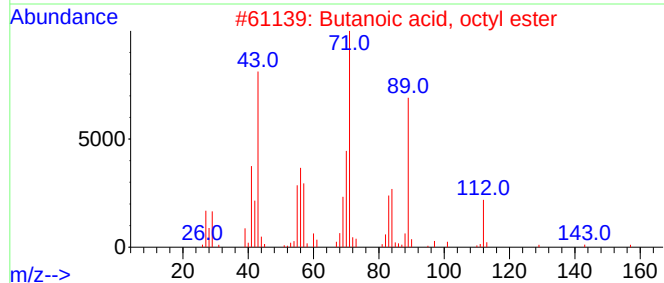
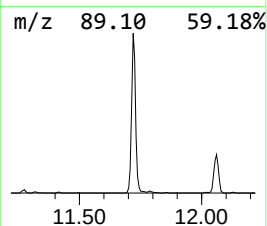
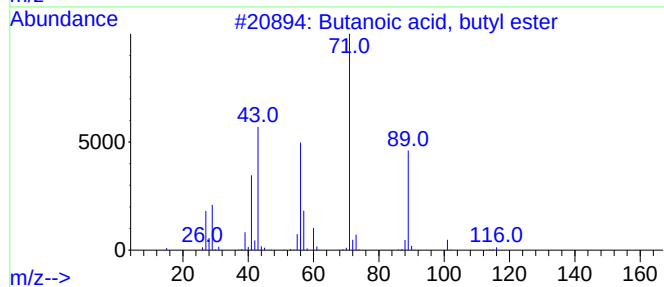
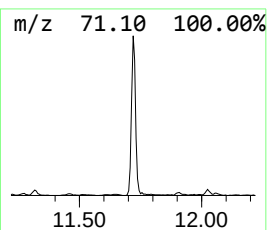
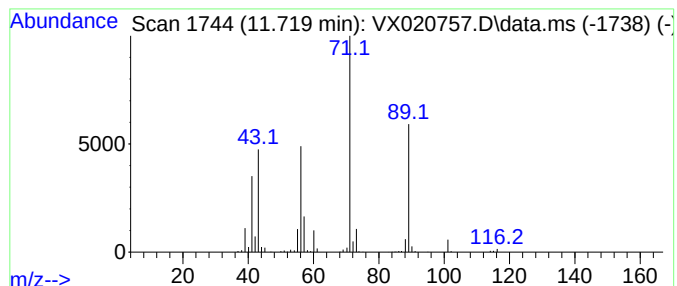
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 4 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.720	6.36 ug/l	213992	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	78
3			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
4			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020757.D
Acq On : 26 Jan 2021 16:41
Operator : JC/SP
Sample : M1189-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41107

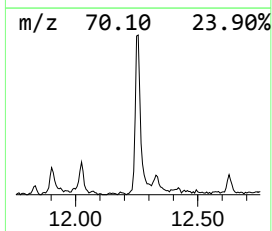
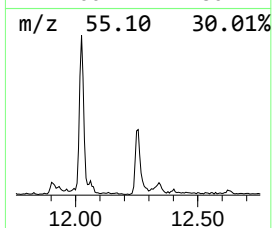
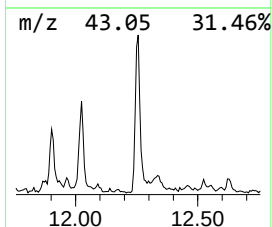
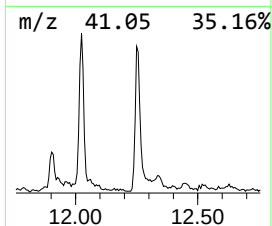
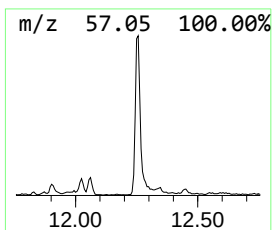
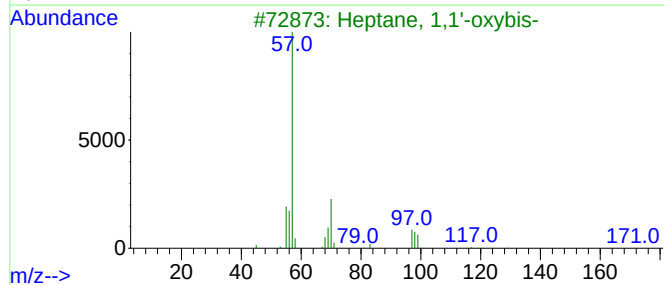
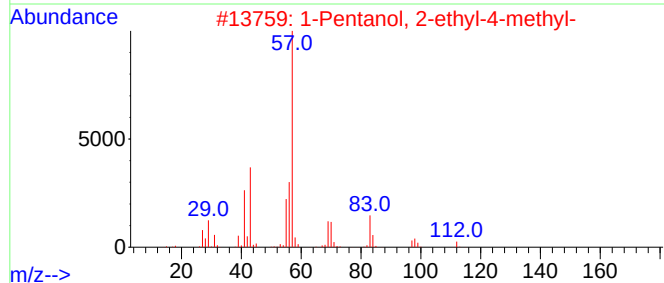
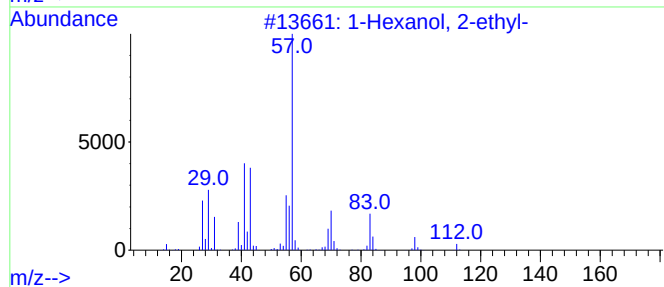
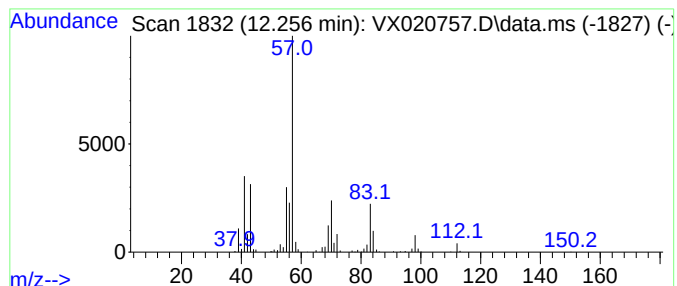
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.256	6.88 ug/l	231428	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	1000365-19-6	47
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020757.D
Acq On : 26 Jan 2021 16:41
Operator : JC/SP
Sample : M1189-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41107

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.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
Propane	1.160	10.8	ug/l	231308	1	5.629	1072860	50.0
Acetaldehyde	1.471	59.4	ug/l	1275500	1	5.629	1072860	50.0
Butanal	4.300	20.7	ug/l	443870	1	5.629	1072860	50.0
Butanoic acid, ...	11.720	6.4	ug/l	213992	4	12.061	1682180	50.0
1-Hexanol, 2-et...	12.256	6.9	ug/l	231428	4	12.061	1682180	50.0