

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX020320\
 Data File : VX014790.D
 Acq On : 03 Feb 2020 12:04
 Operator : JC/SP
 Sample : L1329-19
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-5

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\82X012220W.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	1.070	26	30	43	rBV	992669	1227395	1.95%	0.687%
2	1.466	93	95	126	rBV	39517108	62789572	100.00%	35.132%
3	2.106	193	200	212	rBV	2347673	4068949	6.48%	2.277%
4	2.344	232	239	248	rBV2	22768503	40400028	64.34%	22.605%
5	2.430	248	253	273	rVB	2921090	4737376	7.54%	2.651%
6	4.033	486	516	533	rBV	7776626	36580458	58.26%	20.468%
7	4.332	552	565	580	rBV	1302728	3413171	5.44%	1.910%
8	4.661	609	619	634	rBV	239017	655124	1.04%	0.367%
9	5.490	744	755	766	rBV3	258706	742378	1.18%	0.415%
10	5.649	770	781	799	rVB	457381	1297991	2.07%	0.726%
11	6.051	838	847	855	rBV	293638	754401	1.20%	0.422%
12	6.850	966	978	988	rBV	732647	1740632	2.77%	0.974%
13	6.959	988	996	1009	rVB	794710	1819695	2.90%	1.018%
14	7.282	1042	1049	1059	rBV	562137	1150202	1.83%	0.644%
15	8.709	1275	1283	1289	rBV	1494055	2312268	3.68%	1.294%
16	8.776	1289	1294	1300	rVV	1036709	1548478	2.47%	0.866%
17	9.050	1327	1339	1354	rBV	2902331	4156824	6.62%	2.326%
18	9.575	1421	1425	1433	rVB	795198	1062698	1.69%	0.595%
19	10.105	1507	1512	1523	rVB	1480715	2150222	3.42%	1.203%
20	10.629	1593	1598	1606	rBV	513955	680767	1.08%	0.381%
21	11.129	1675	1680	1686	rBV	1192386	1545905	2.46%	0.865%
22	12.074	1831	1835	1842	rVB	1533259	1902526	3.03%	1.065%
23	12.263	1861	1866	1877	rBV	1546854	1985208	3.16%	1.111%

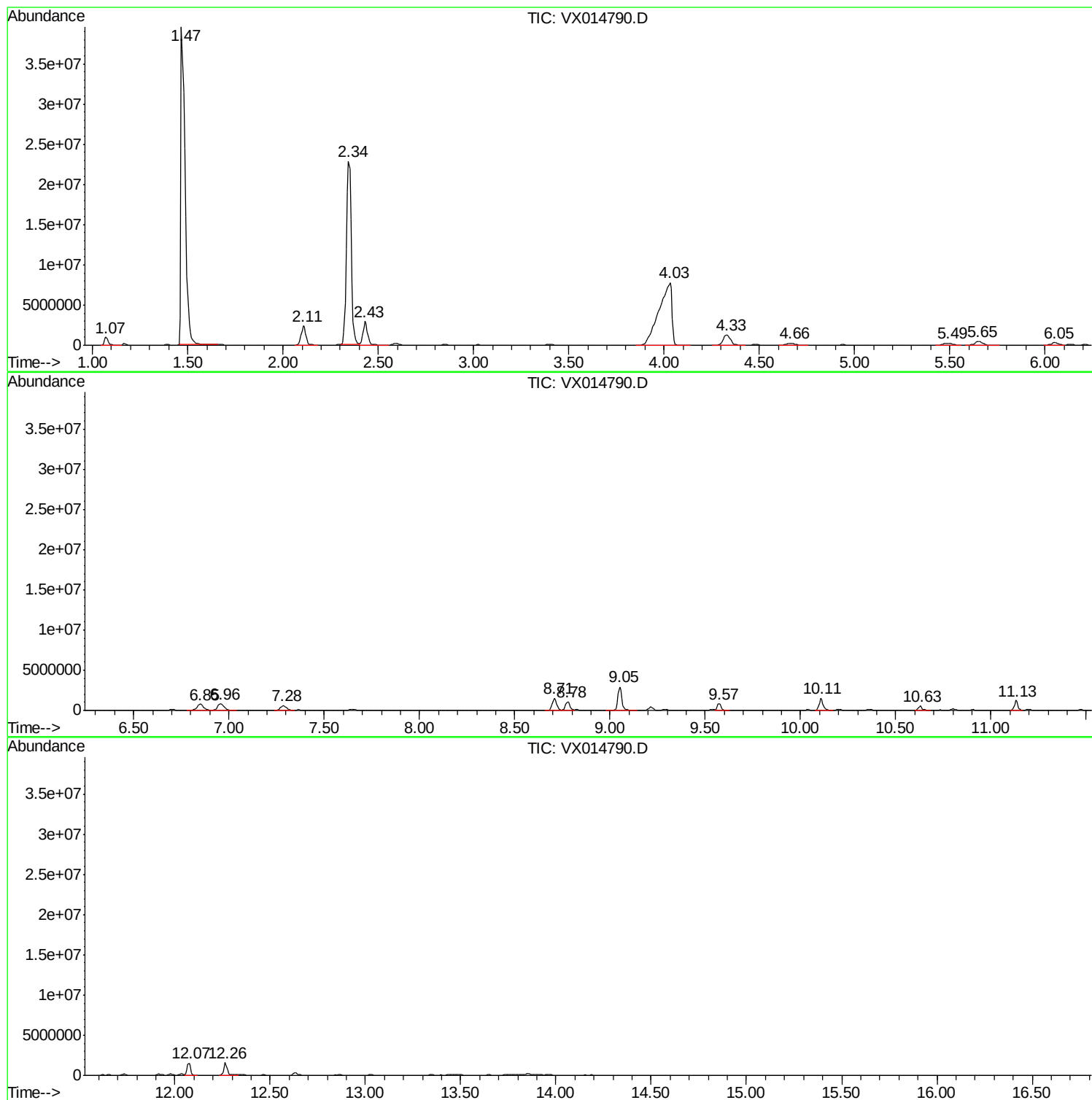
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Quant Title : SW846 8260

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



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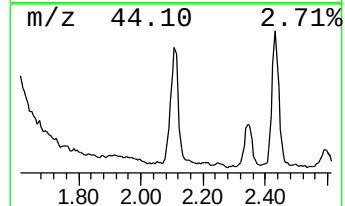
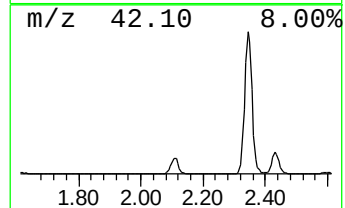
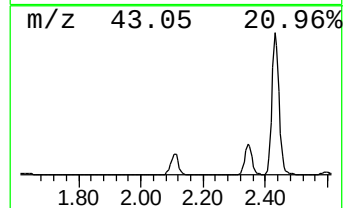
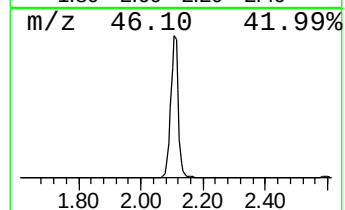
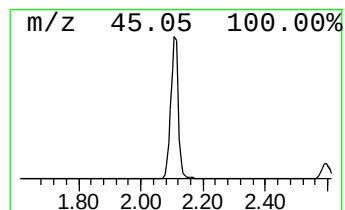
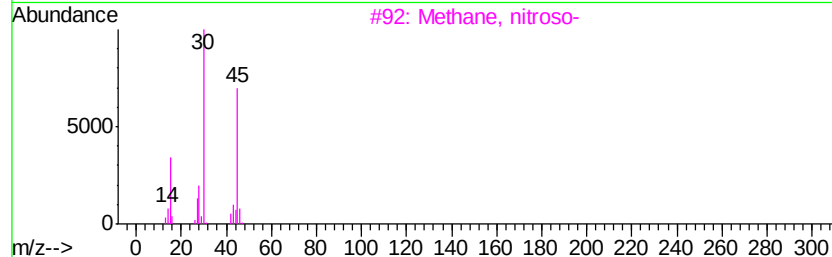
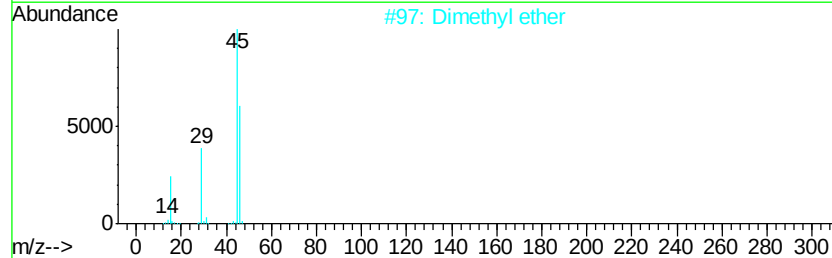
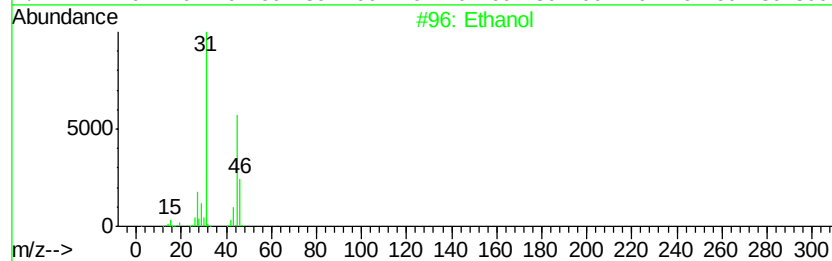
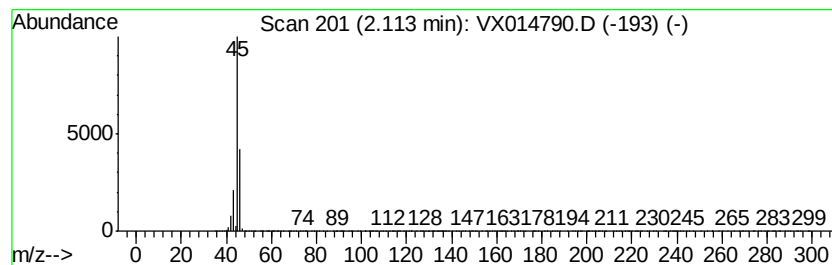
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.11	156.74 ug/l	4068950	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	78
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



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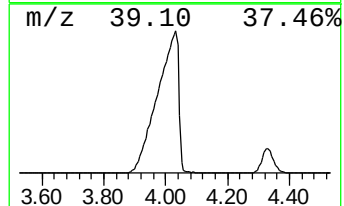
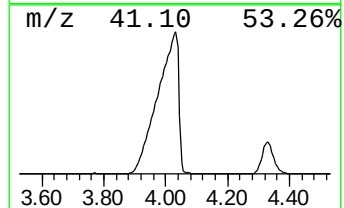
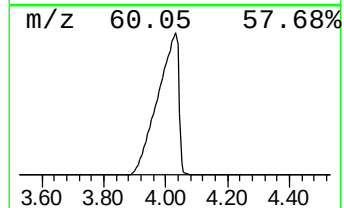
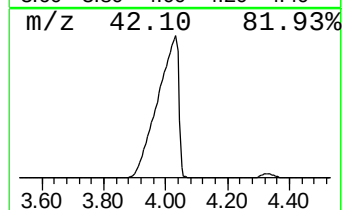
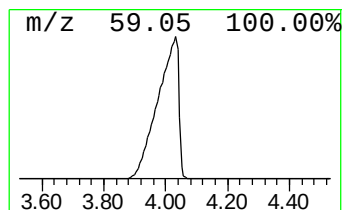
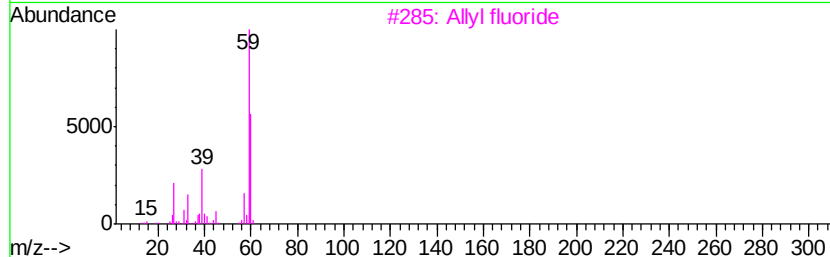
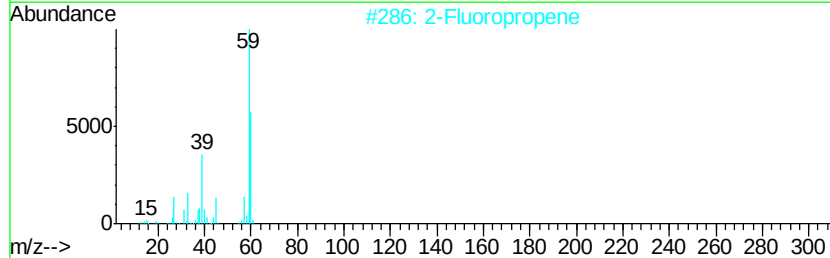
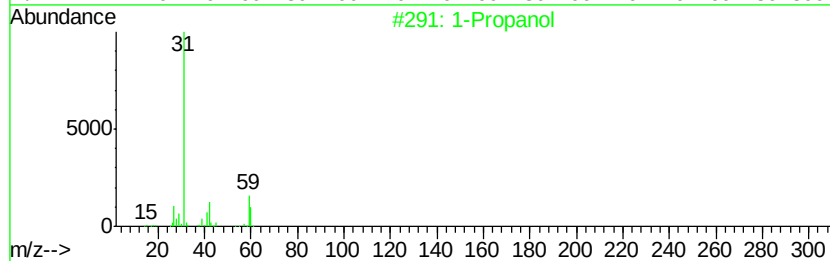
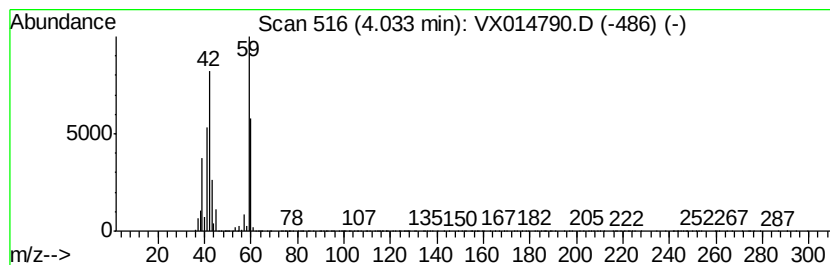
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.03	1409.12 ug/l	36580500	Pentafluorobenzene	5.65

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	43
3		Allyl fluoride	60	C3H5F	000818-92-8	38
4		Cyclopropane	42	C3H6	000075-19-4	16
5		Acetaldoxime	59	C2H5NO	000107-29-9	7



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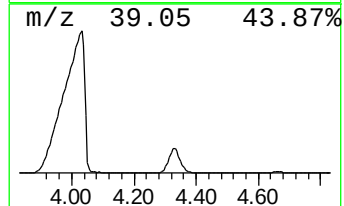
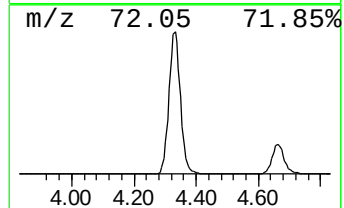
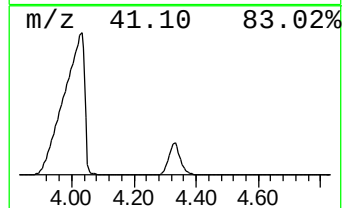
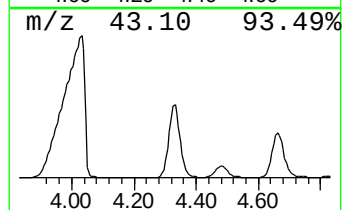
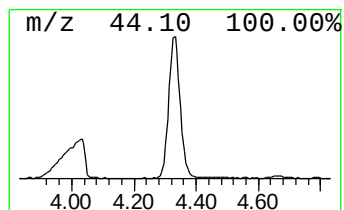
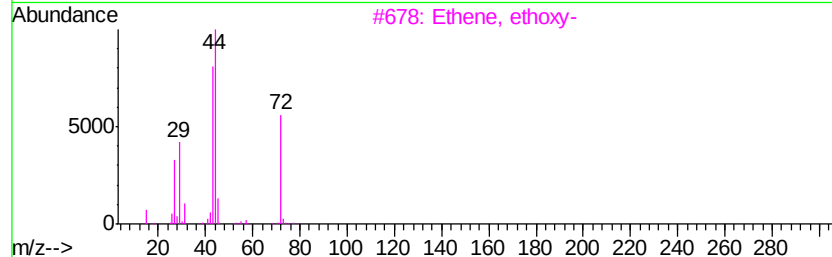
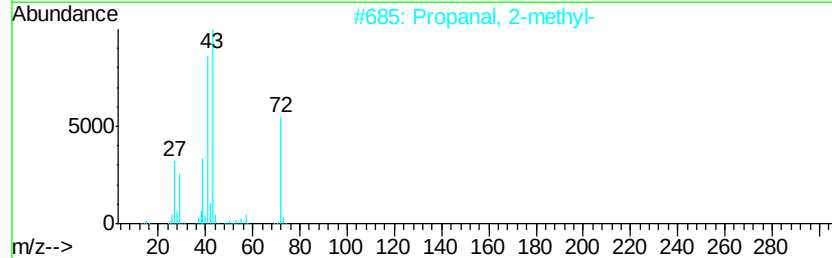
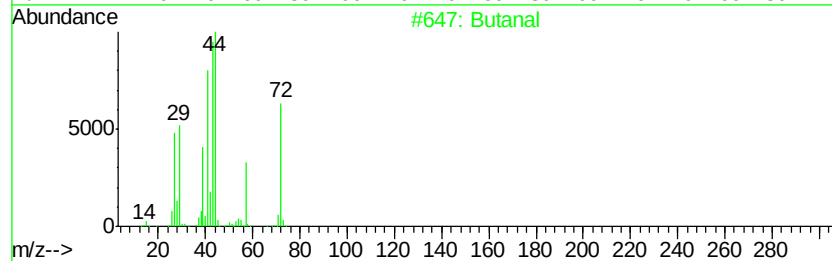
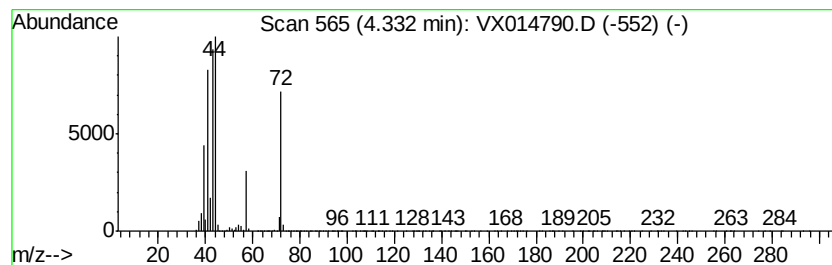
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Peak Number 5 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	131.48 ug/l	3413170	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal		72	C4H8O	000123-72-8	94
2	Propanal, 2-methyl-		72	C4H8O	000078-84-2	52
3	Ethene, ethoxy-		72	C4H8O	000109-92-2	49
4	1-Propene, 3-methoxy-		72	C4H8O	000627-40-7	32
5	Isobutylene epoxide		72	C4H8O	000558-30-5	22



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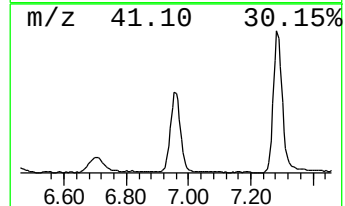
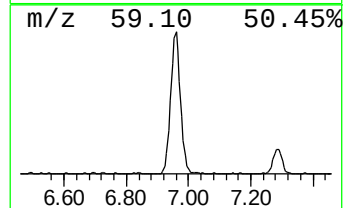
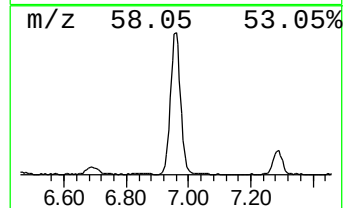
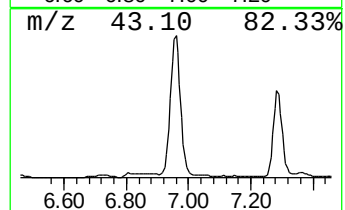
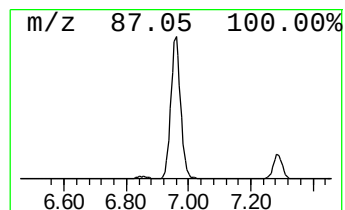
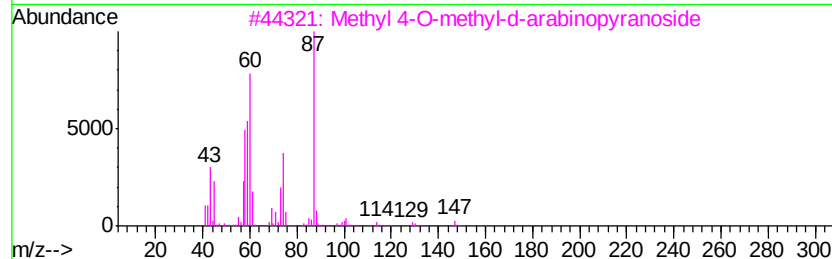
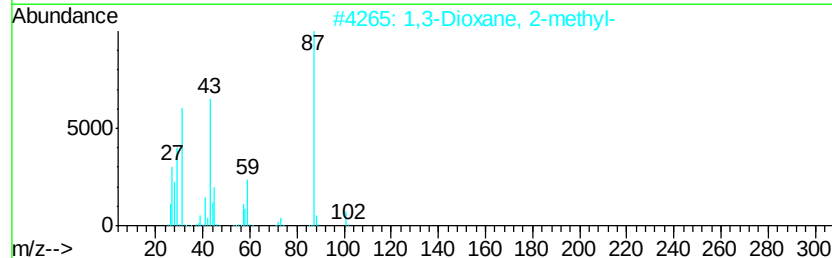
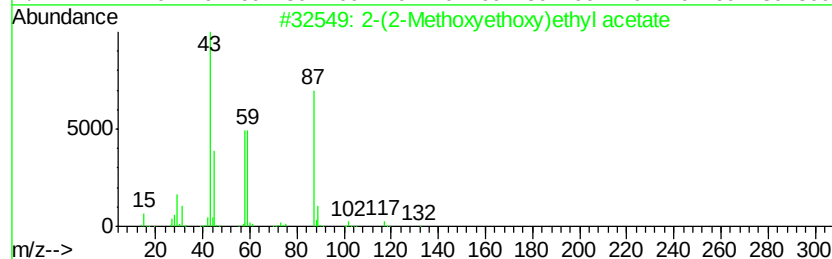
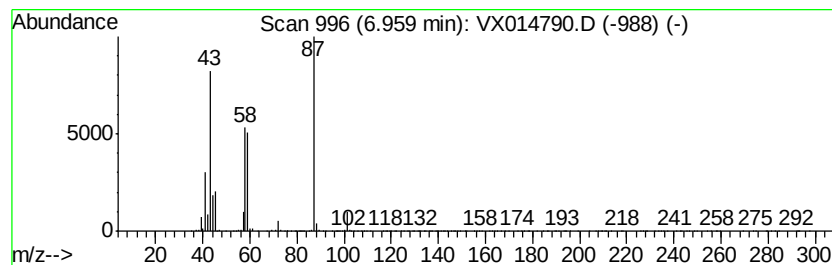
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Peak Number 6 unknown hydrocarbon6.96 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.96	52.27 ug/l	1819700	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	45
2		1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	42
3		Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
4		Monomethyl malonate	118	C4H6O4	016695-14-0	33
5		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	25



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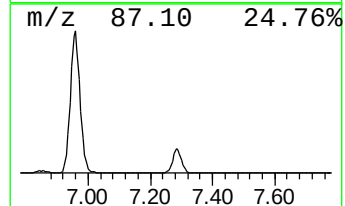
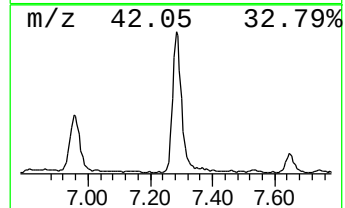
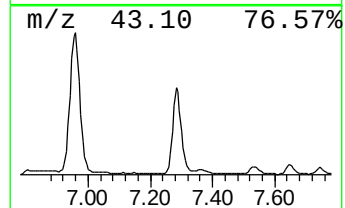
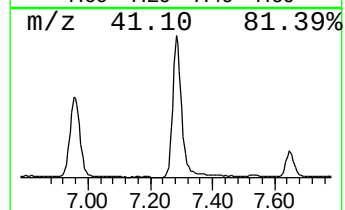
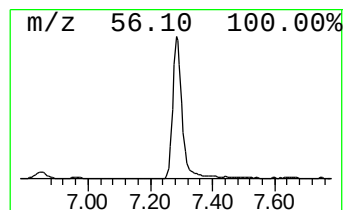
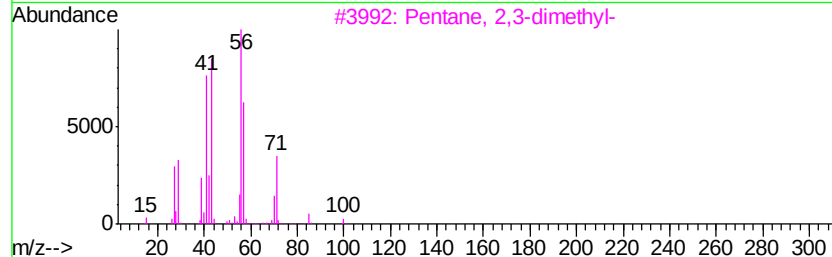
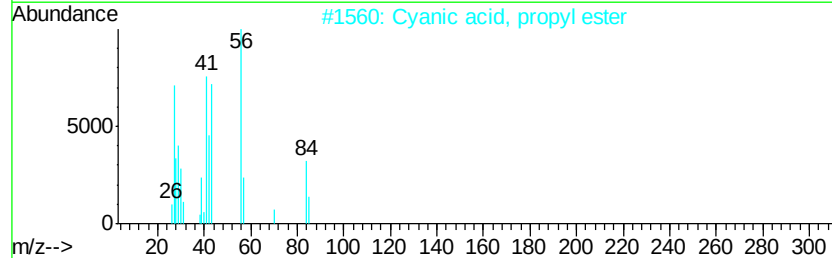
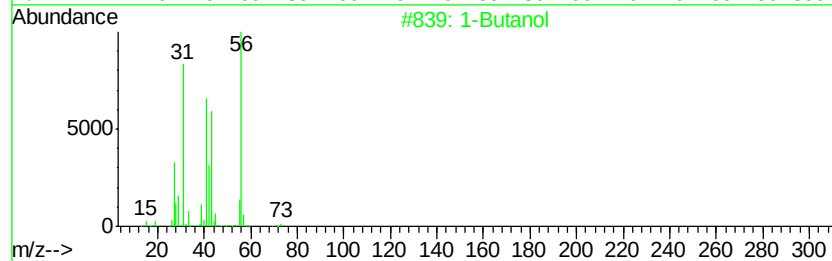
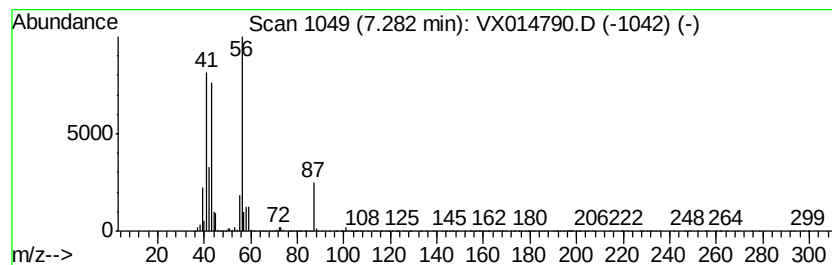
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TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Butanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.28	33.04 ug/l	1150200	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol	74	C4H10O	000071-36-3	68
2		Cyanoic acid, propyl ester	85	C4H7NO	001768-36-1	40
3		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	40
4		1-Hexanol	102	C6H14O	000111-27-3	36
5		2-Azetidinecarboxylic acid	101	C4H7NO2	002517-04-6	35



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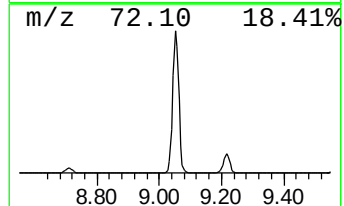
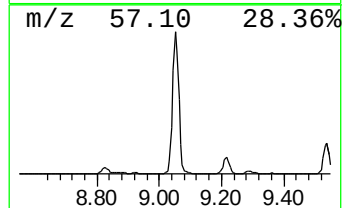
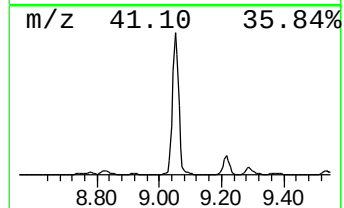
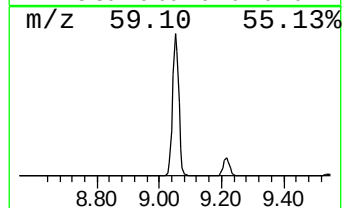
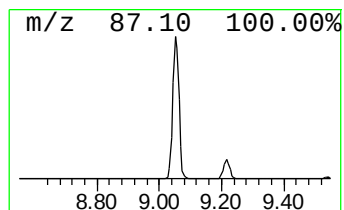
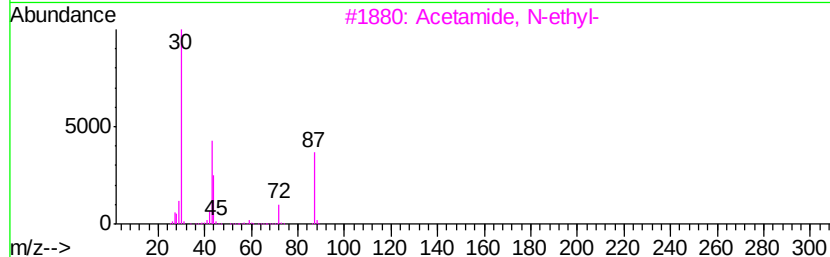
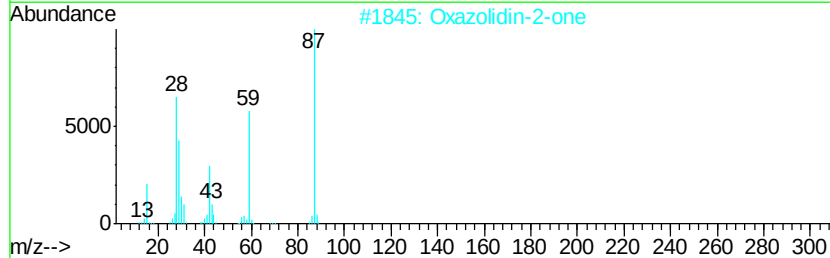
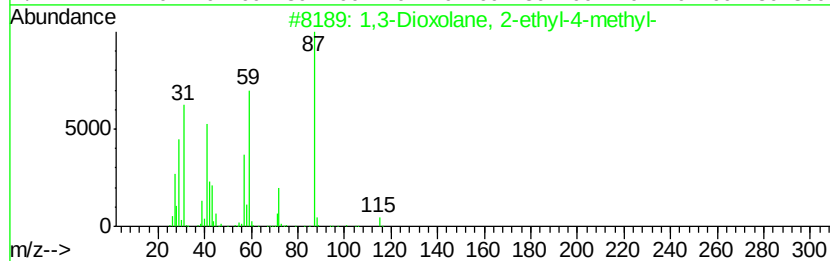
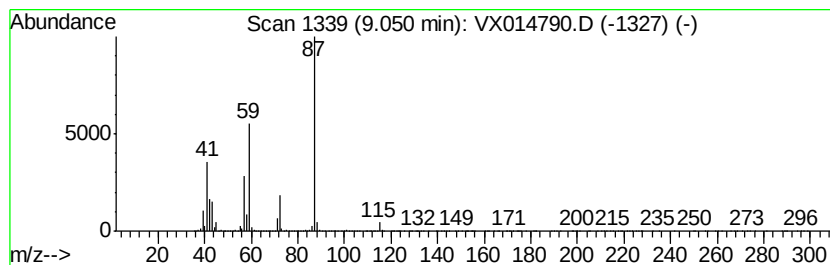
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 8 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	96.66 ug/l	4156820	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	72
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53
4		2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5		Ethanol, 2-[2-(2-methoxyethoxy)e...	206	C9H18O5	003610-27-3	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX020320\
Data File : VX014790.D
Acq On : 03 Feb 2020 12:04
Operator : JC/SP
Sample : L1329-19
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-5

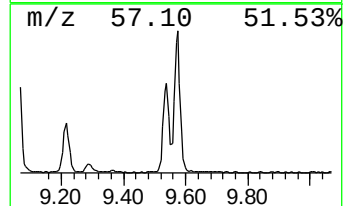
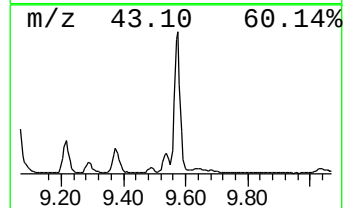
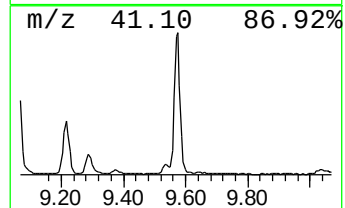
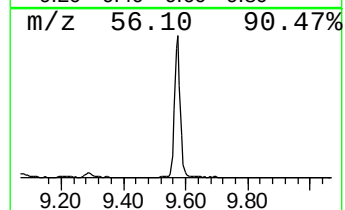
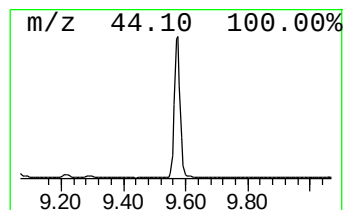
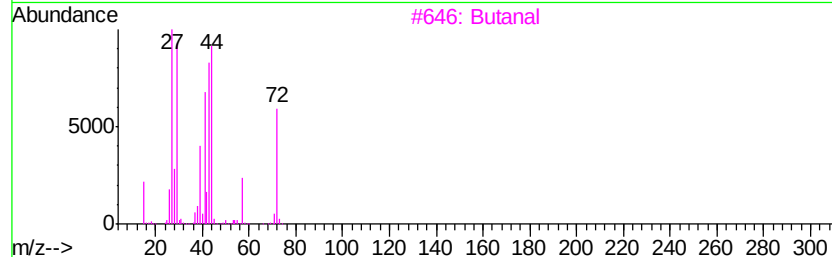
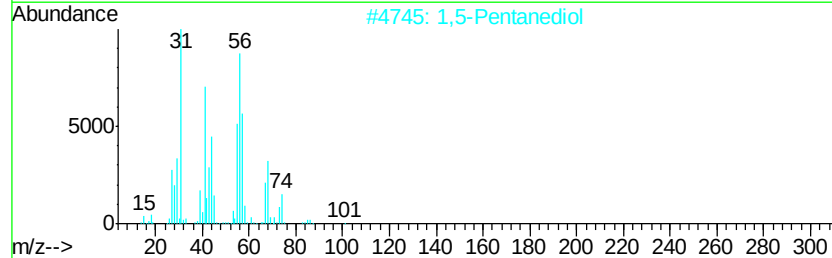
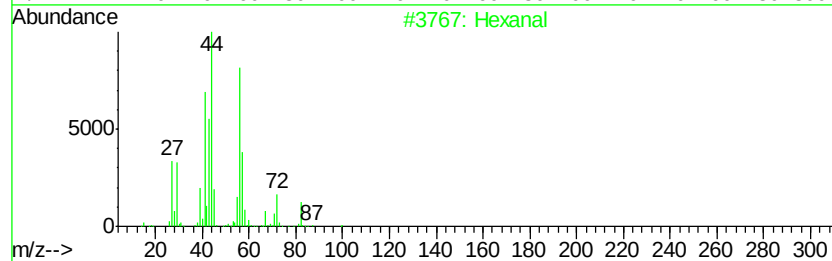
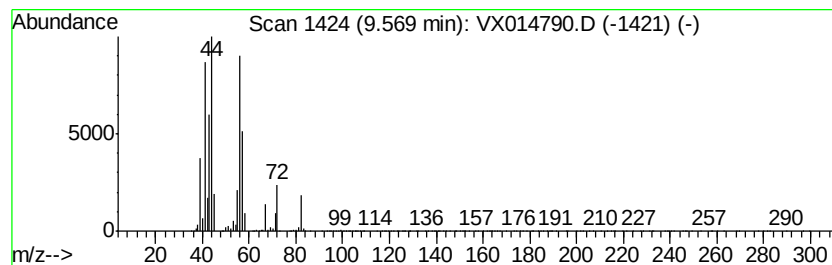
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 9 Hexanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	24.71 ug/l	1062700	Chlorobenzene-d5	10.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal		100	C6H12O	000066-25-1	91
2	1,5-Pentanediol		104	C5H12O2	000111-29-5	28
3	Butanal		72	C4H8O	000123-72-8	27
4	Aziridine, 2-methyl-		57	C3H7N	000075-55-8	25
5	Butanal, 3-methyl-		86	C5H10O	000590-86-3	16



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX020320\
Data File : VX014790.D
Acq On : 03 Feb 2020 12:04
Operator : JC/SP
Sample : L1329-19
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
COMP-5

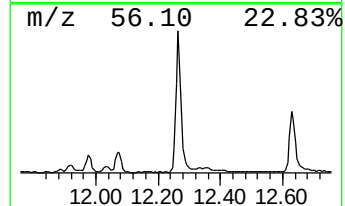
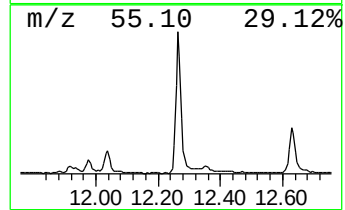
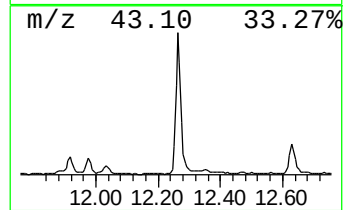
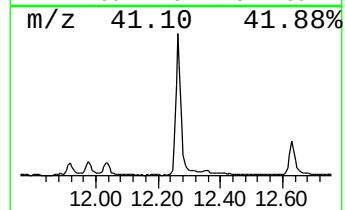
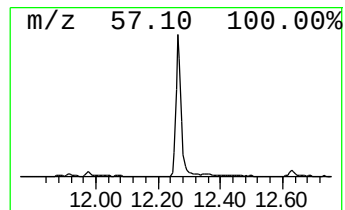
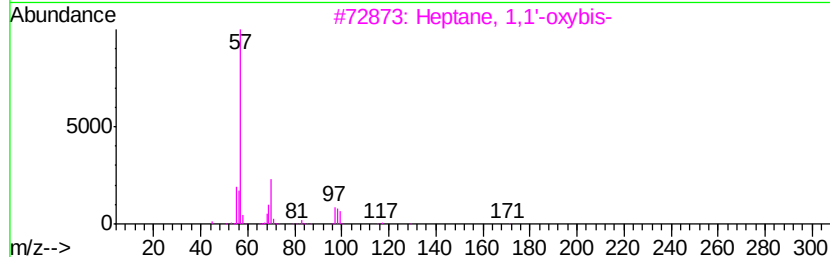
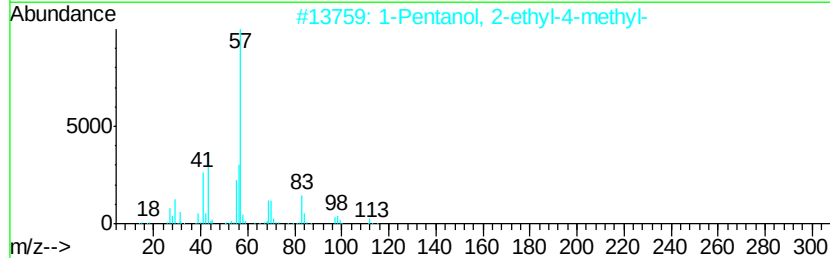
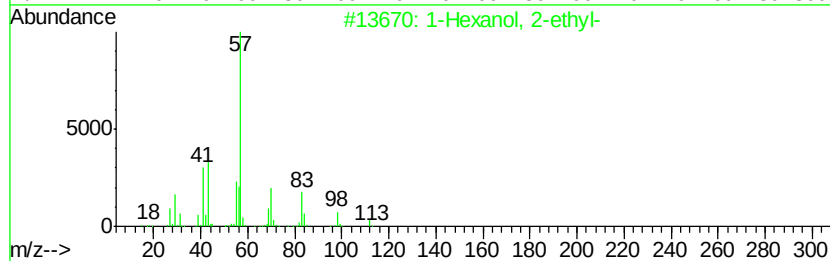
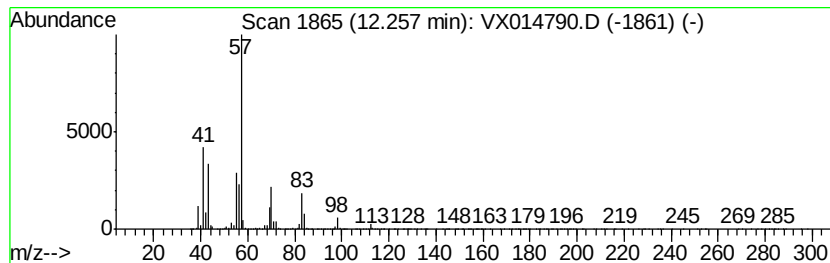
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	52.17 ug/l	1985210	1,4-Dichlorobenzene-d4	12.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020320\
Data File : VX014790.D
Acq On : 03 Feb 2020 12:04
Operator : JC/SP
Sample : L1329-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.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
Ethanol	2.11	156.7	ug/l	4068950	1	5.65	1297990	50.0
1-Propanol	4.03	1409.1	ug/l	36580500	1	5.65	1297990	50.0
Butanal	4.33	131.5	ug/l	3413170	1	5.65	1297990	50.0
unknown hydrocarb...	6.96	52.3	ug/l	1819700	2	6.85	1740630	50.0
1-Butanol	7.28	33.0	ug/l	1150200	2	6.85	1740630	50.0
1,3-Dioxolane, 2-...	9.05	96.7	ug/l	4156820	3	10.11	2150220	50.0
Hexanal	9.57	24.7	ug/l	1062700	3	10.11	2150220	50.0
1-Hexanol, 2-ethyl-	12.26	52.2	ug/l	1985210	4	12.07	1902530	50.0