

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073123\
 Data File : VX036713.D
 Acq On : 31 Jul 2023 12:23
 Operator : JC/MD
 Sample : 03806-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ORA-1694

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\82X072123W.M

Title : SW846 8260

Signal : TIC: VX036713.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	72	rBV	967353	1218159	4.52%	1.778%
2	2.294	186	198	210	rBV	9500840	26941180	100.00%	39.314%
3	3.891	442	460	481	rBV	1580217	5164832	19.17%	7.537%
4	4.233	505	516	529	rBV	219741	586064	2.18%	0.855%
5	5.385	694	705	720	rVB	95964	278383	1.03%	0.406%
6	5.550	720	732	747	rVB	159544	453358	1.68%	0.662%
7	5.958	788	799	814	rBV	101793	275842	1.02%	0.403%
8	6.763	919	931	941	rBV	254041	622426	2.31%	0.908%
9	6.873	941	949	963	rVB	188971	454411	1.69%	0.663%
10	7.208	995	1004	1014	rBV2	156911	337973	1.25%	0.493%
11	8.647	1233	1240	1248	rBV	534747	835759	3.10%	1.220%
12	9.000	1290	1298	1318	rBV	10795708	17298918	64.21%	25.243%
13	9.165	1318	1325	1334	rBV	8162769	11971935	44.44%	17.470%
14	10.055	1465	1471	1484	rBV	540651	893893	3.32%	1.304%
15	11.079	1634	1639	1645	rBV	433771	543243	2.02%	0.793%
16	12.024	1789	1794	1805	rVB	491826	652223	2.42%	0.952%

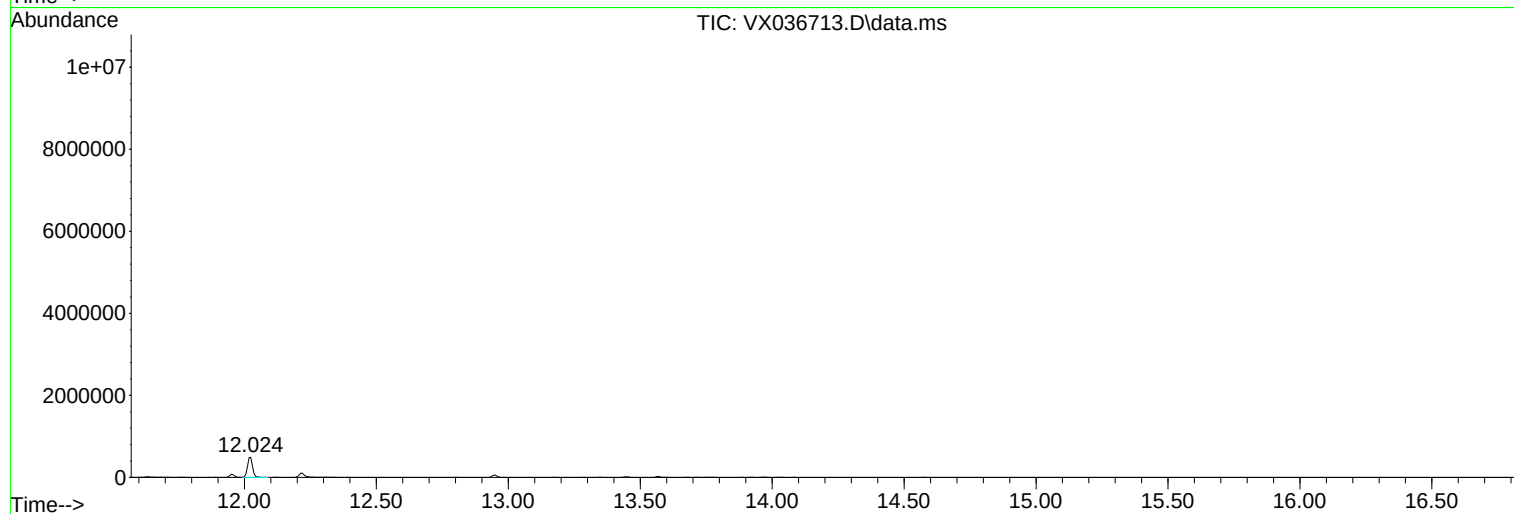
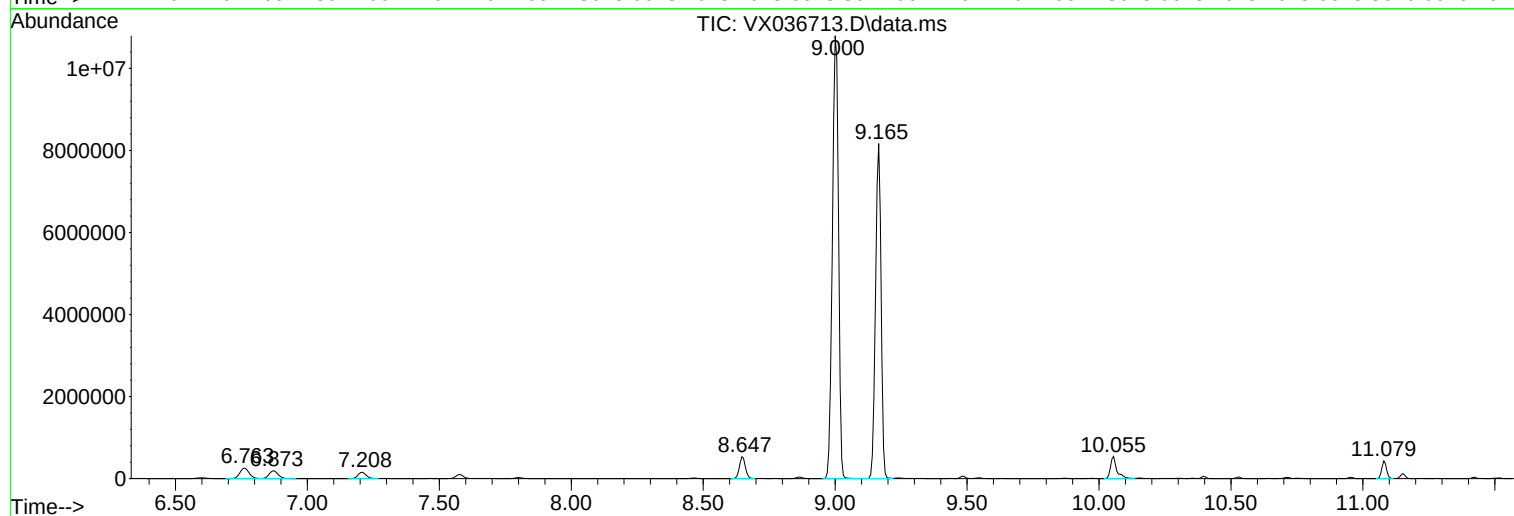
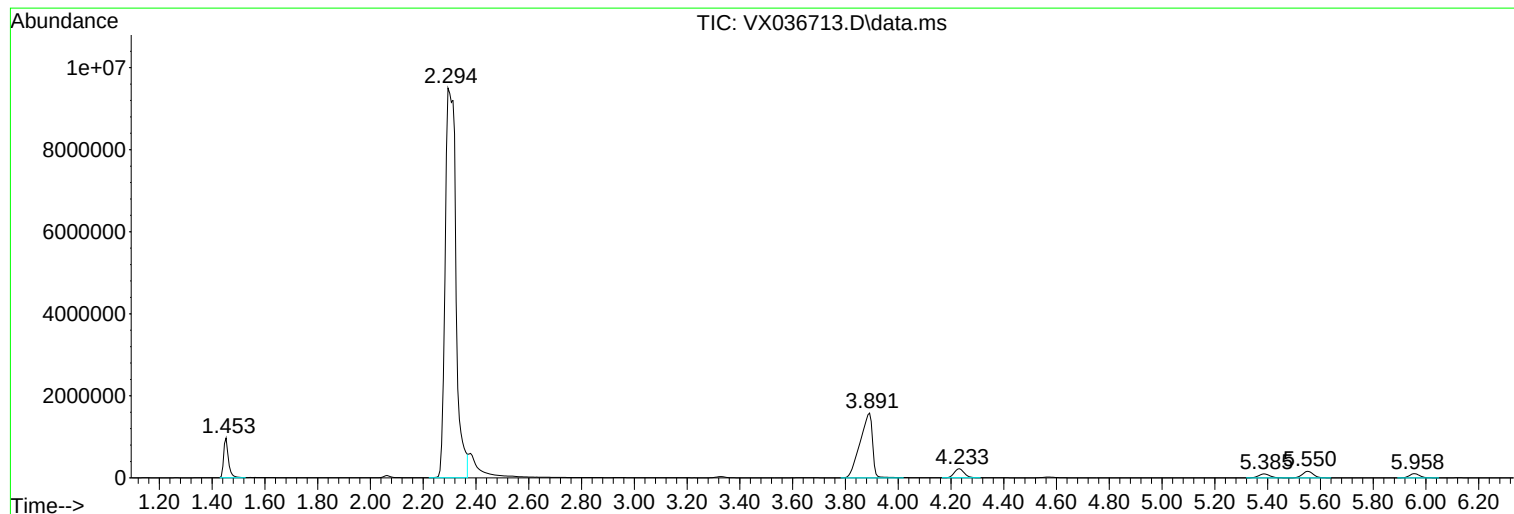
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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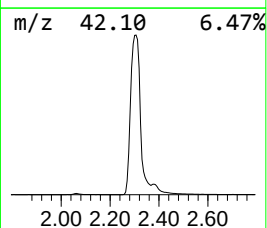
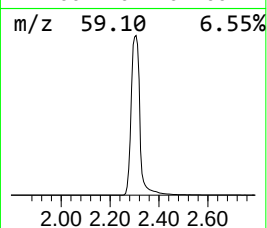
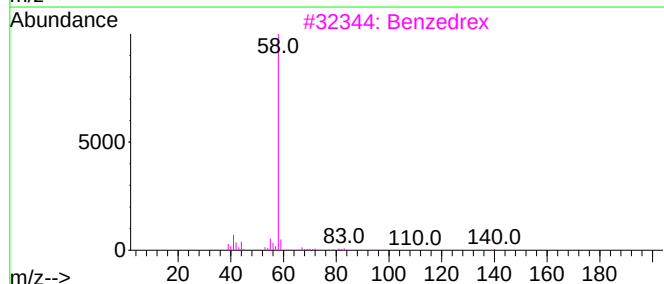
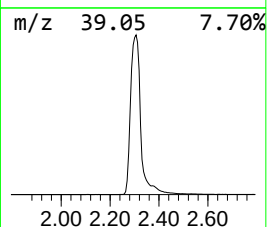
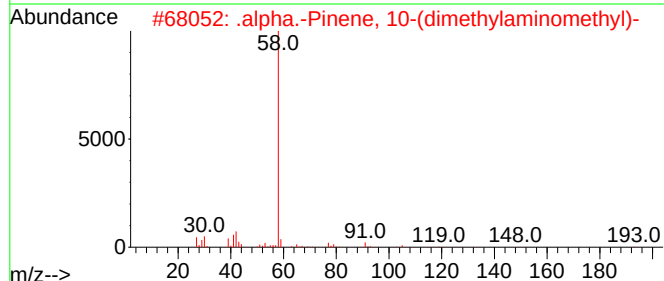
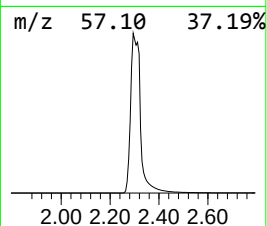
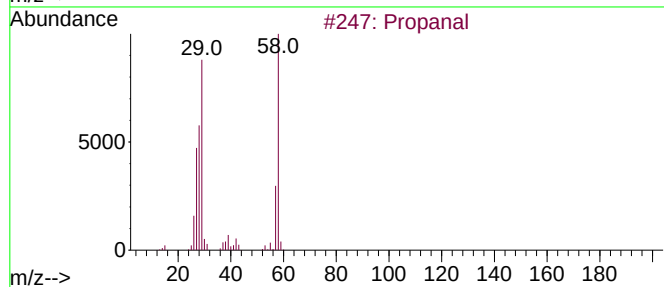
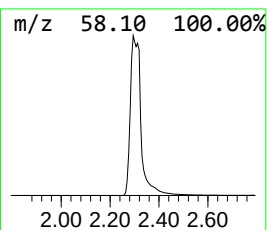
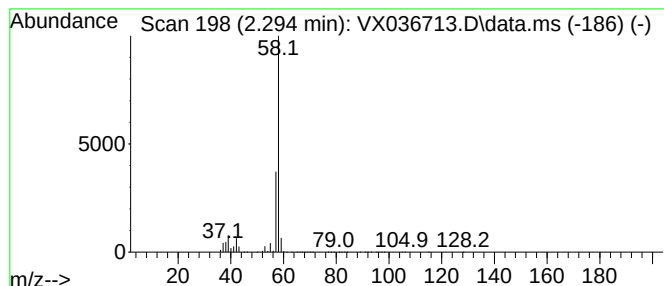
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	2971.29 ug/l	26941200	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	80
2			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
3			Benzedrex	155	C10H21N	000101-40-6	9
4			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
5			Propylene oxide	58	C3H6O	000075-56-9	5



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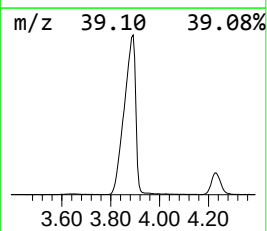
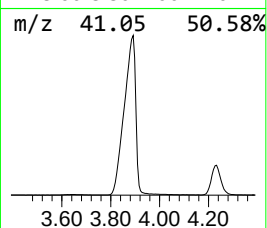
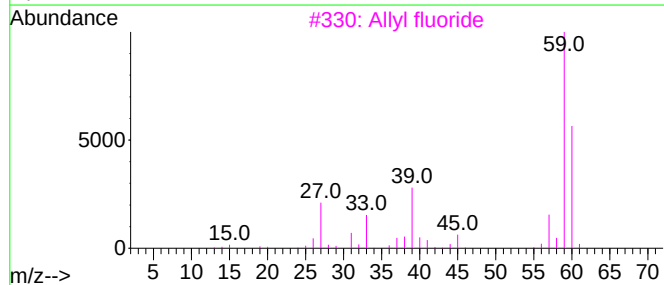
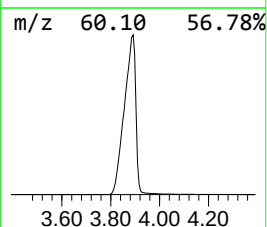
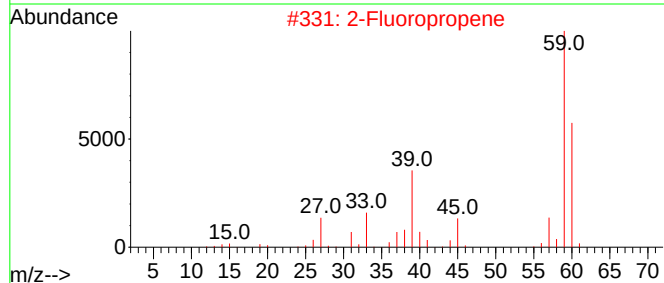
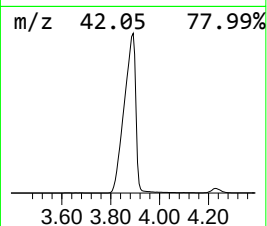
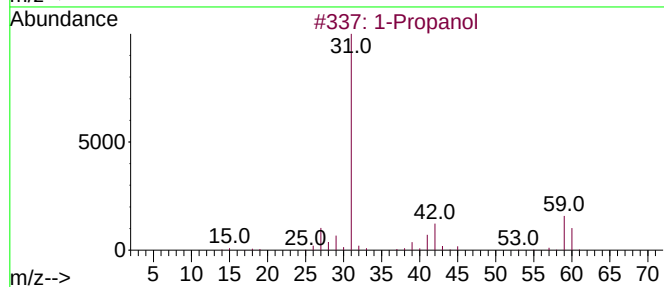
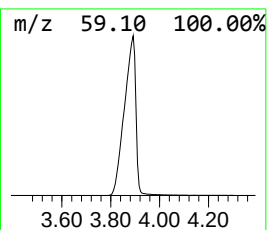
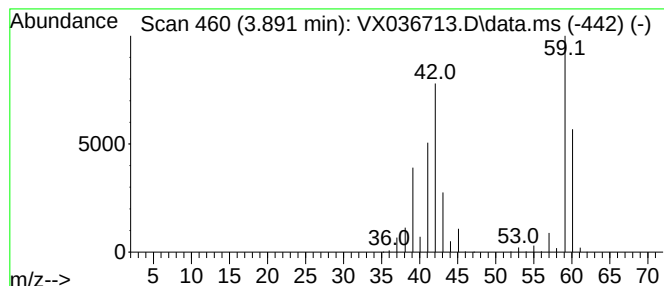
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.891	569.62 ug/l	5164830	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	64
2	2-Fluoropropene			60	C3H5F	001184-60-7	47
3	Allyl fluoride			60	C3H5F	000818-92-8	38
4	Cyclopropane			42	C3H6	000075-19-4	32
5	Formamidoxime			60	CH4N2O	000624-82-8	9



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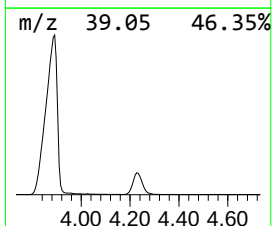
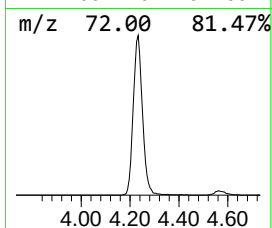
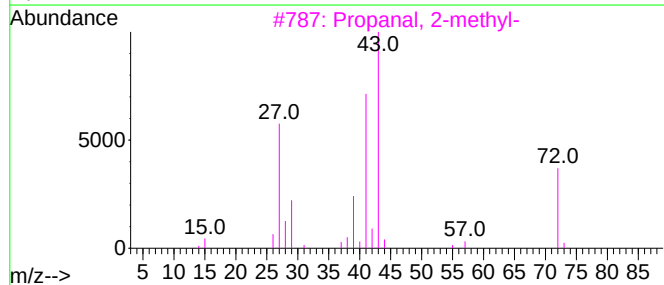
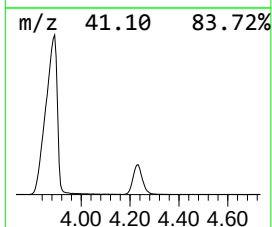
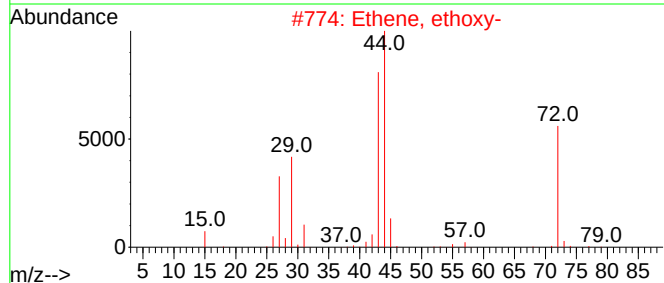
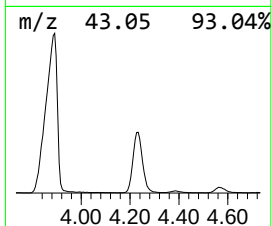
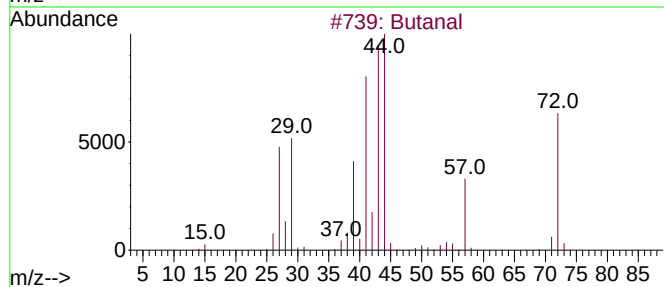
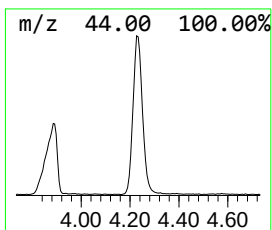
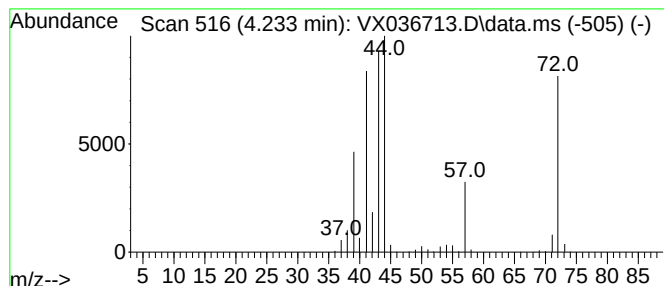
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Peak Number 4 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	64.64 ug/l	586064	Pentafluorobenzene	5.550

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	43
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38



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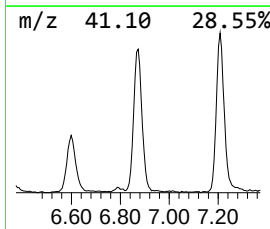
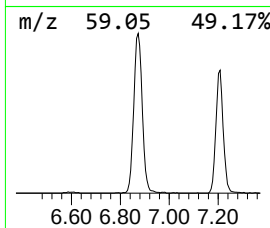
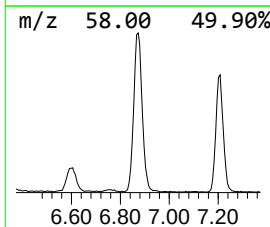
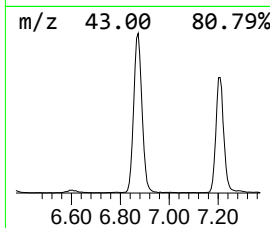
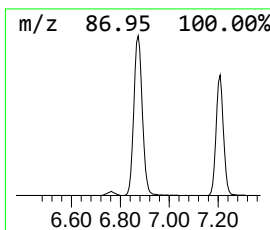
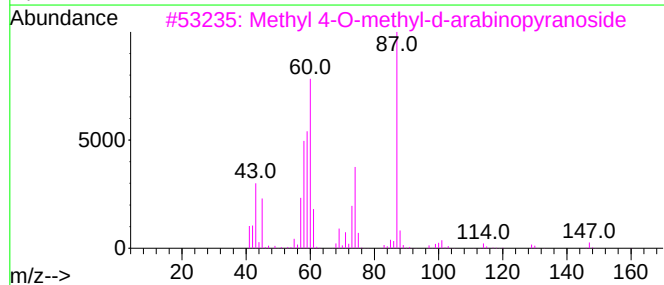
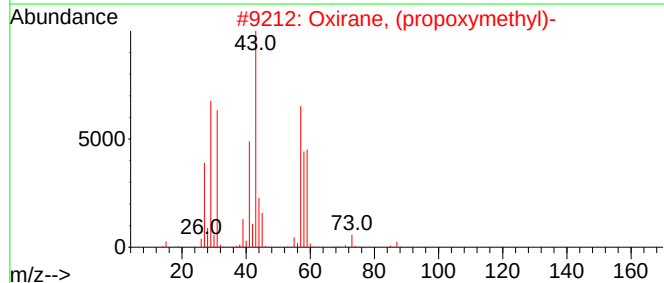
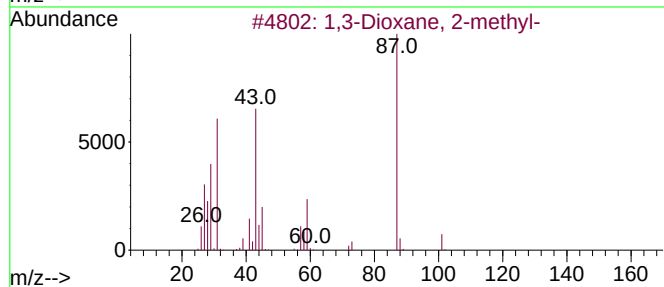
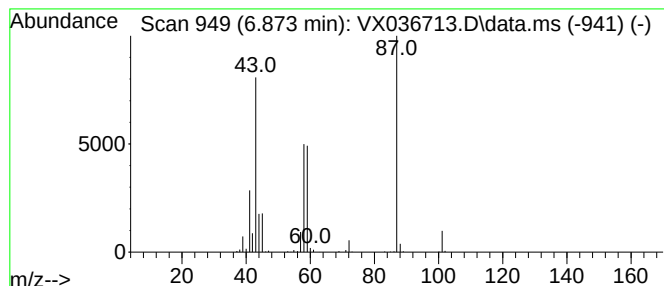
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TIC Integration Parameters: LSCINT.P

Peak Number 5 1,3-Dioxane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.873	36.50 ug/l	454411	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	50
2			Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	38
3			Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
4			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	38
5			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	33



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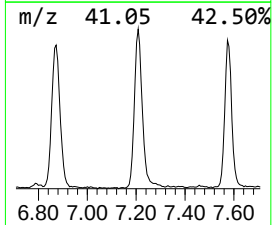
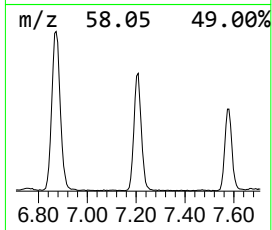
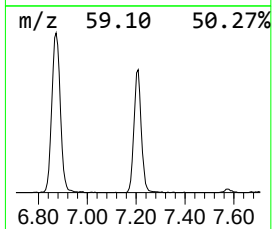
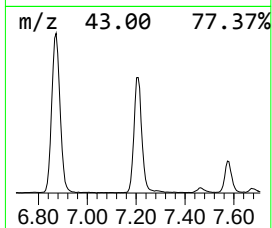
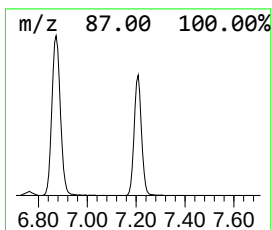
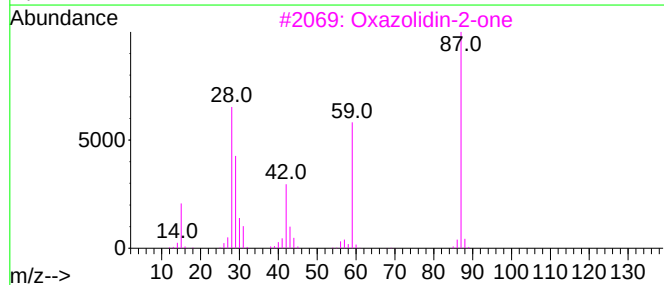
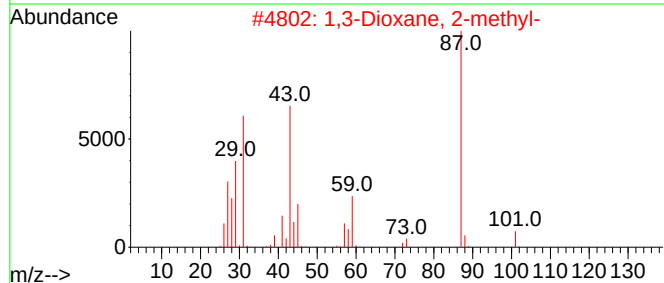
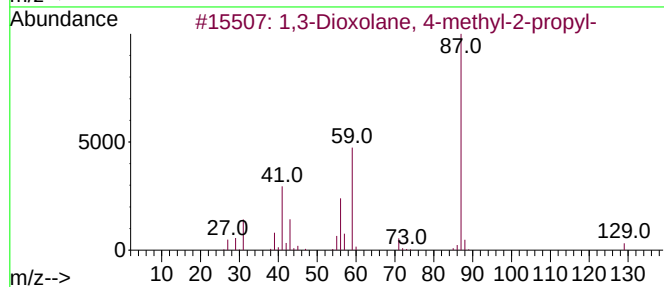
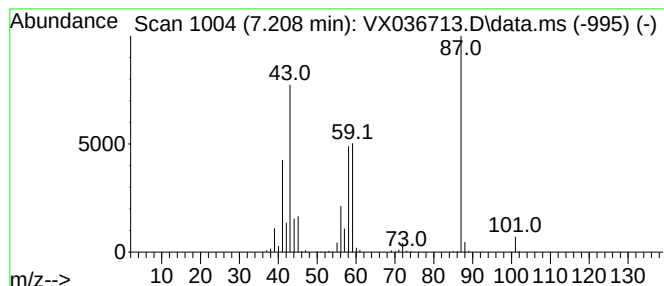
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	27.15 ug/l	337973	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	53	
2	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	50	
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	47	
4	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	45	
5	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	38	



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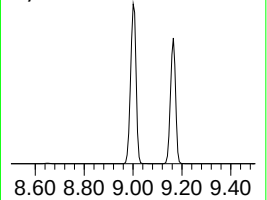
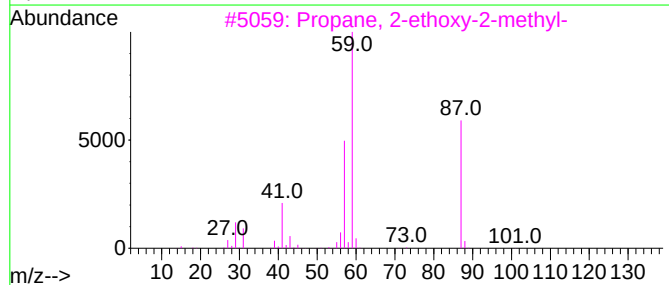
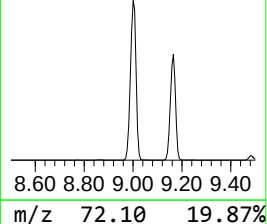
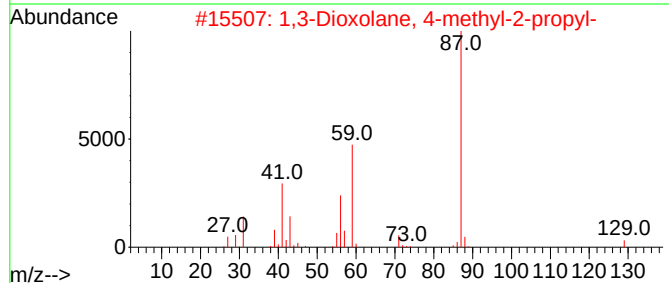
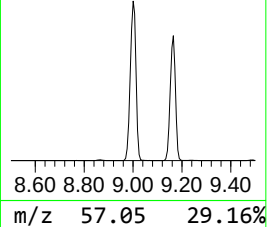
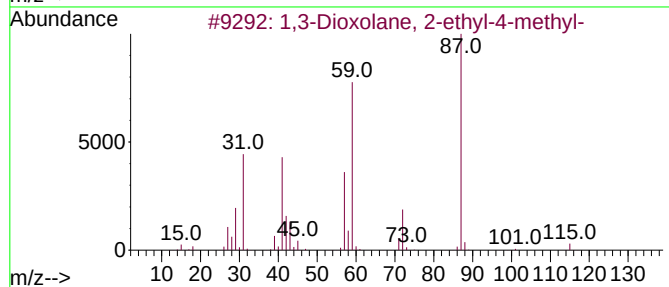
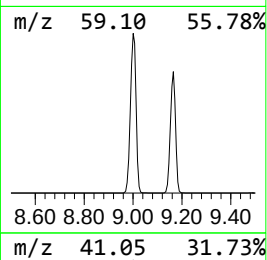
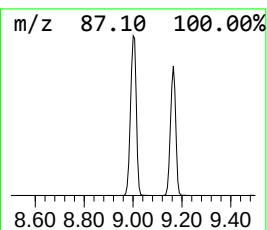
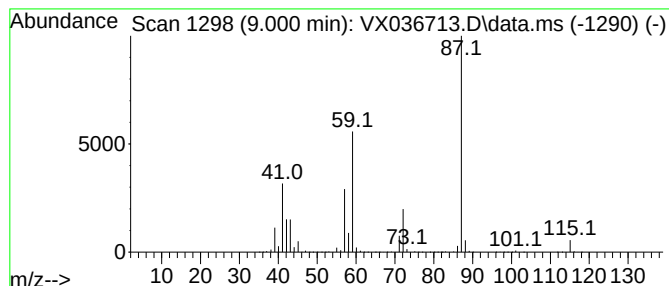
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.000	967.62 ug/l	17298900	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	90
2			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64
3			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	59
4			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	58
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073123\
Data File : VX036713.D
Acq On : 31 Jul 2023 12:23
Operator : JC/MD
Sample : 03806-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1694

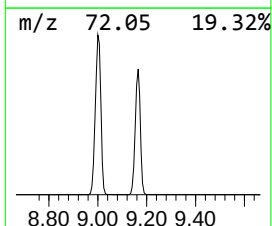
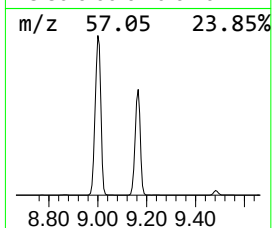
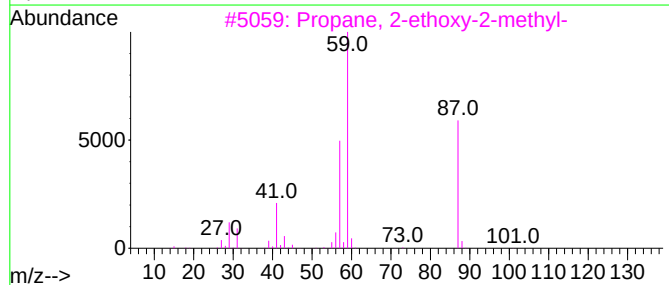
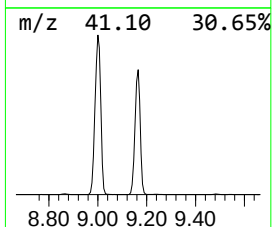
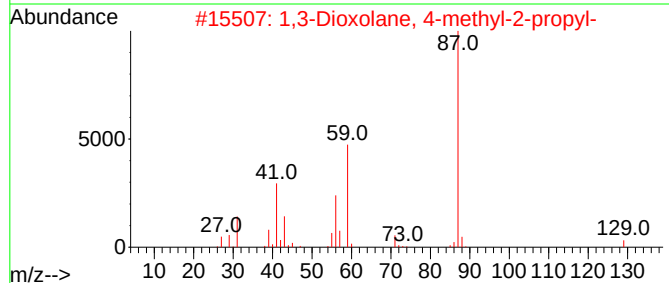
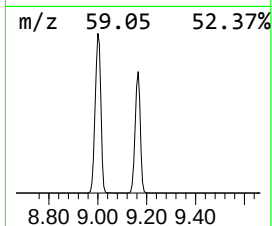
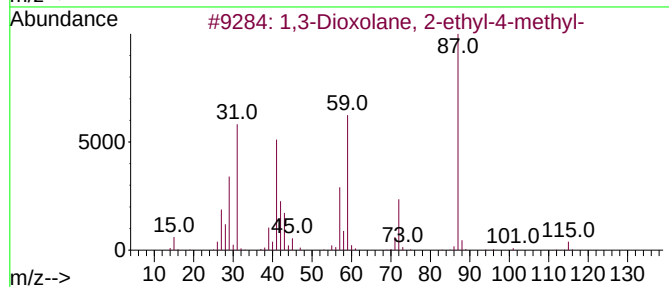
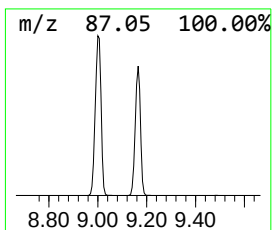
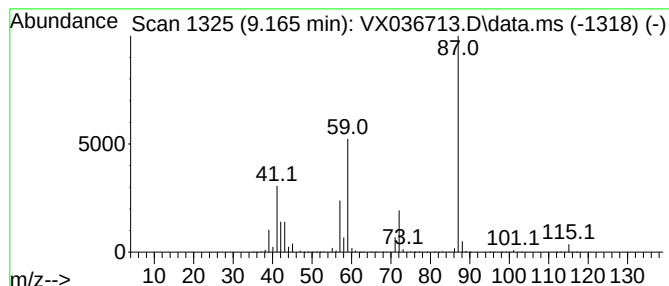
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Propane, 2-ethoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.165	669.65 ug/l	11971900	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91		
2	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64		
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	59		
4	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	56		
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073123\
Data File : VX036713.D
Acq On : 31 Jul 2023 12:23
Operator : JC/MD
Sample : 03806-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1694

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal	2.294	2971.3	ug/l	26941200	1	5.550	453358	50.0
1-Propanol	3.891	569.6	ug/l	5164830	1	5.550	453358	50.0
Butanal	4.233	64.6	ug/l	586064	1	5.550	453358	50.0
1,3-Dioxane, 2-...	6.873	36.5	ug/l	454411	2	6.763	622426	50.0
1,3-Dioxolane, ...	7.208	27.1	ug/l	337973	2	6.763	622426	50.0
1,3-Dioxolane, ...	9.000	967.6	ug/l	17298900	3	10.055	893893	50.0
Propane, 2-etho...	9.165	669.6	ug/l	11971900	3	10.055	893893	50.0