

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102523\
 Data File : VX038486.D
 Acq On : 25 Oct 2023 17:39
 Operator : JC/MD
 Sample : 05036-02 100X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BUR-1282

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\82X100523W.M

Title : SW846 8260

Signal : TIC: VX038486.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	73	rBV	1893075	2207807	100.00%	27.779%
2	2.050	151	158	171	rBV	36969	61623	2.79%	0.775%
3	2.379	204	212	224	rBV	42671	73417	3.33%	0.924%
4	4.233	508	516	532	rBV3	17797	50156	2.27%	0.631%
5	5.385	693	705	721	rBV	108382	318346	14.42%	4.005%
6	5.556	721	733	751	rVV	167587	474497	21.49%	5.970%
7	5.830	769	778	789	rBV	23783	66681	3.02%	0.839%
8	5.958	789	799	815	rVB	112277	291328	13.20%	3.666%
9	6.763	921	931	948	rBV	269697	641353	29.05%	8.070%
10	8.647	1234	1240	1250	rBV	552384	898983	40.72%	11.311%
11	10.055	1465	1471	1485	rBV	632431	870780	39.44%	10.956%
12	10.311	1505	1513	1524	rBV	257491	344325	15.60%	4.332%
13	11.079	1634	1639	1647	rBV	541374	700801	31.74%	8.818%
14	12.024	1788	1794	1803	rVB	713402	947635	42.92%	11.923%

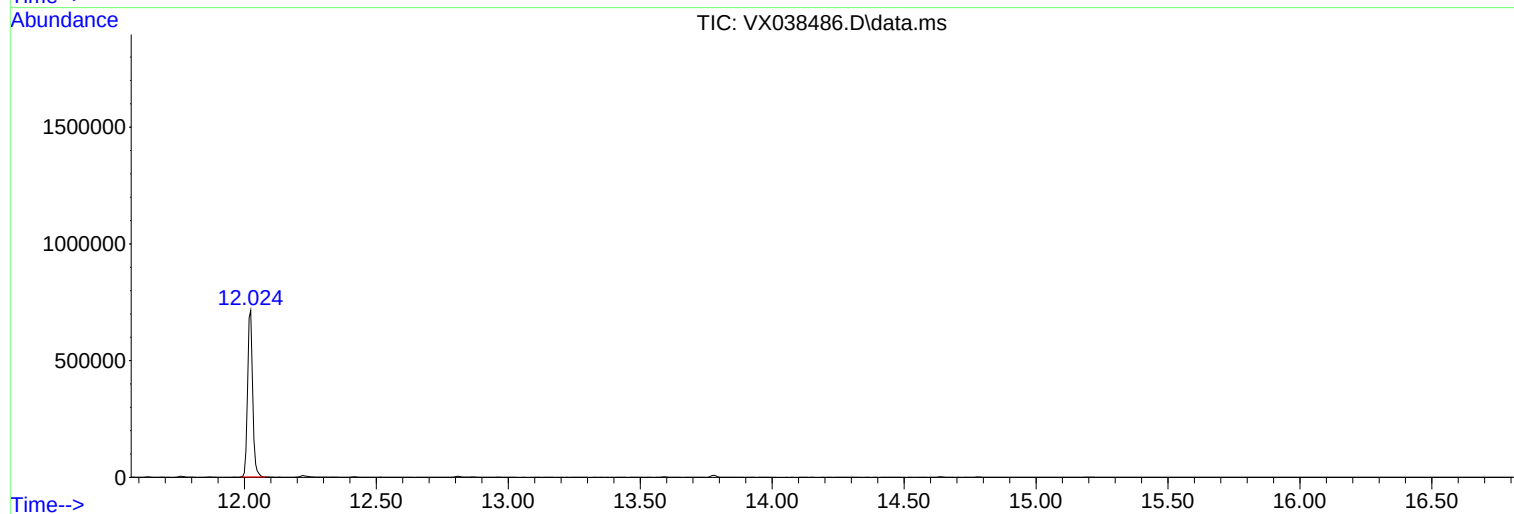
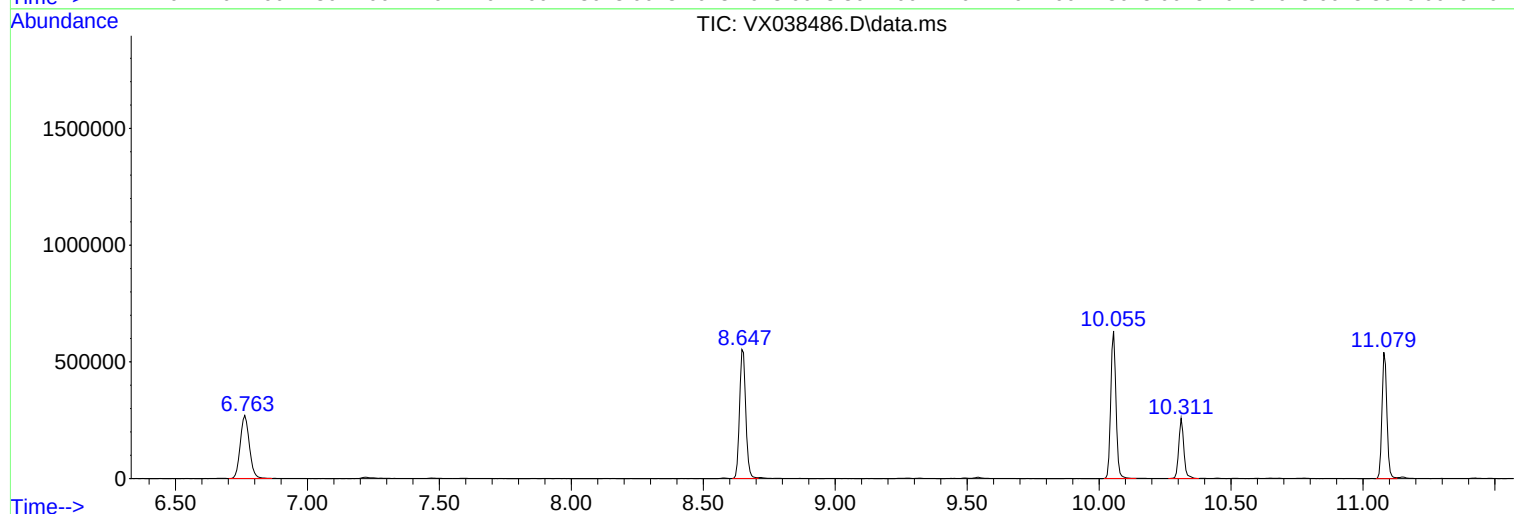
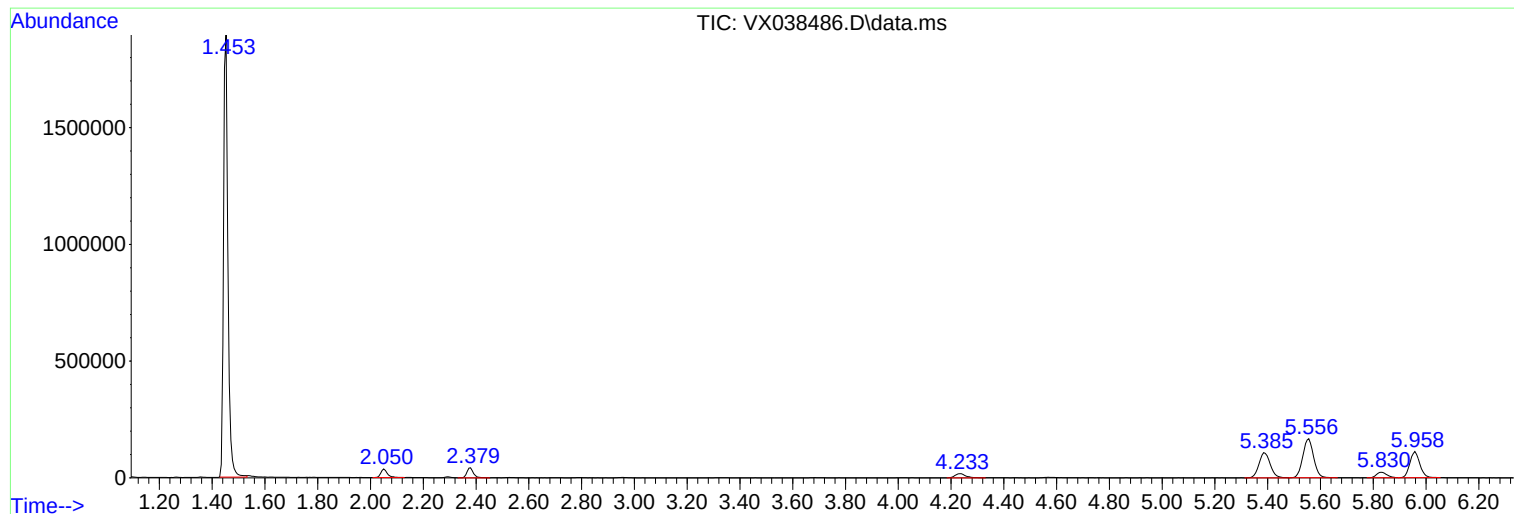
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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



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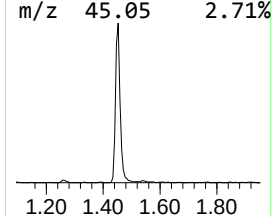
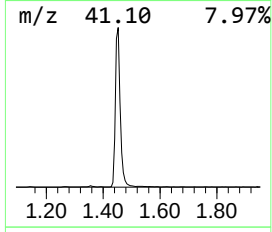
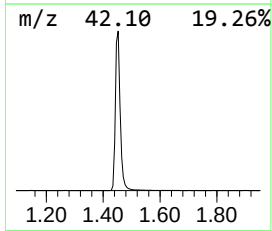
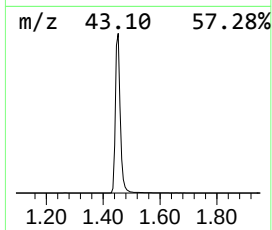
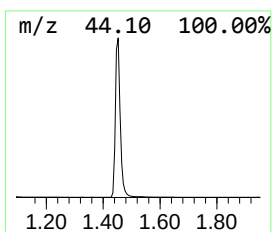
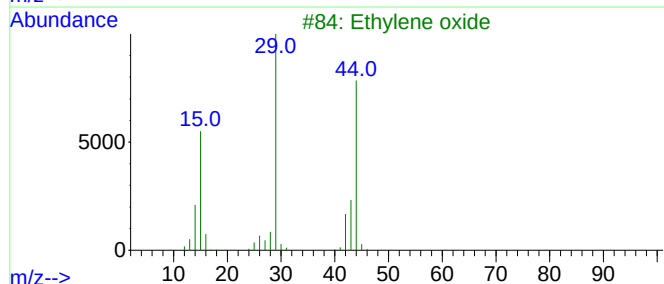
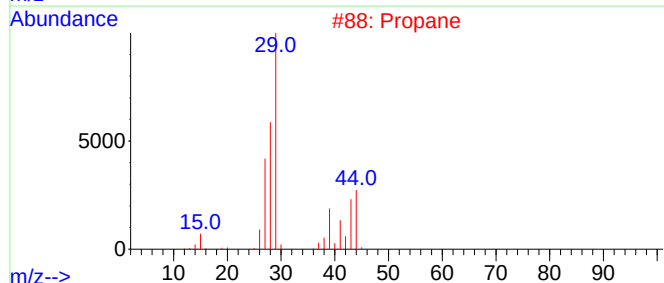
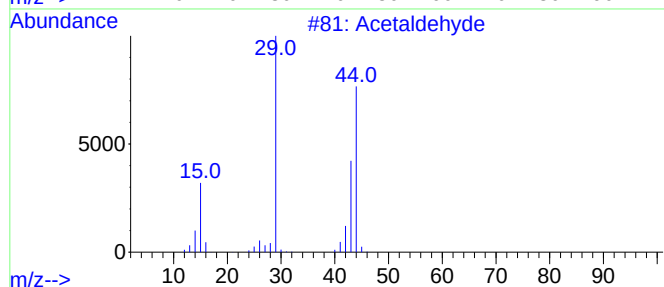
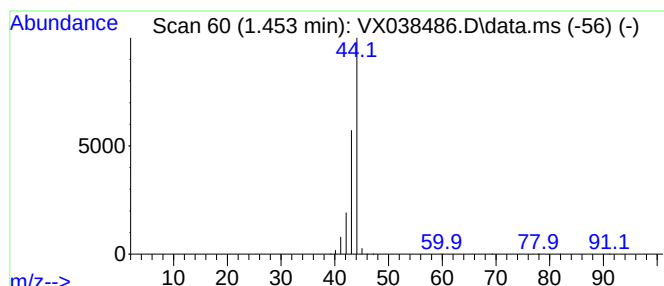
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	232.65 ug/l	2207810	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
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			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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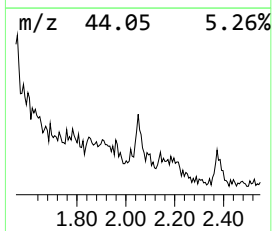
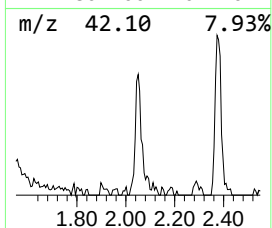
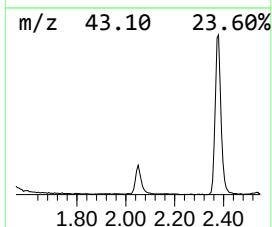
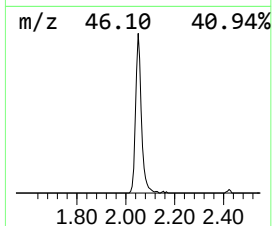
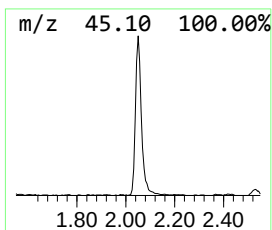
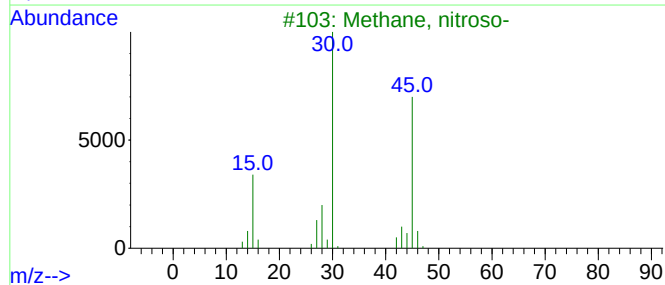
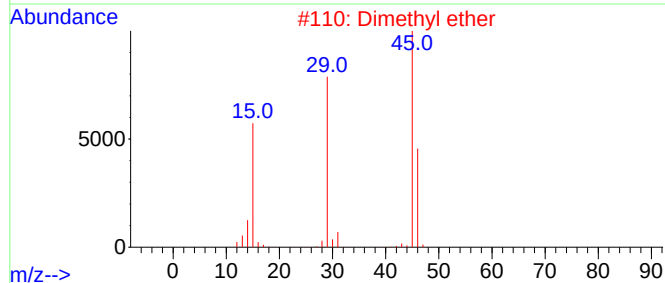
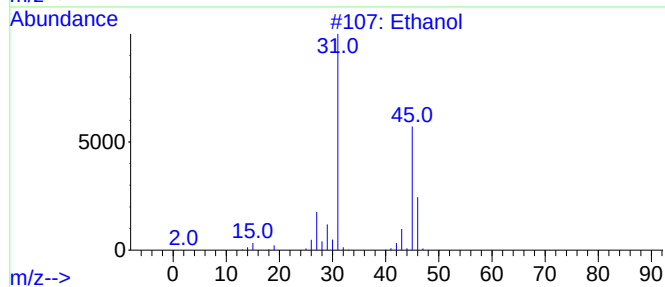
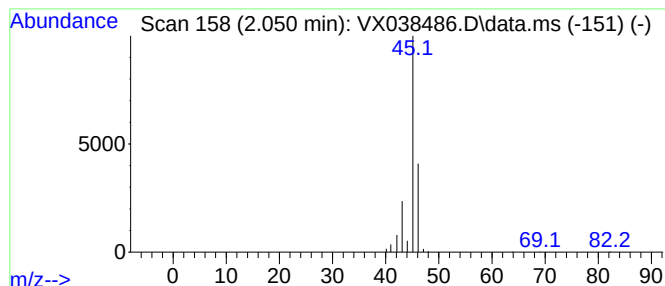
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	6.49 ug/l	61623	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	74
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			Propanedioic acid, dihydroxy-	136	C3H4O6	000560-27-0	4



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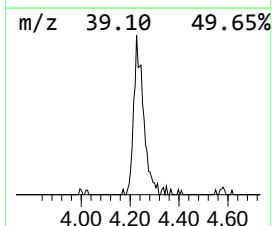
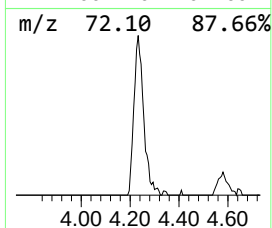
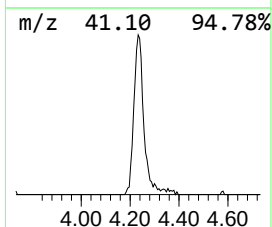
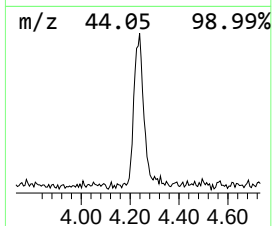
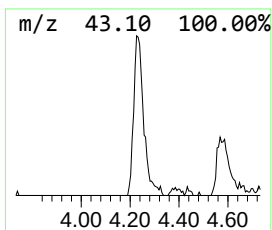
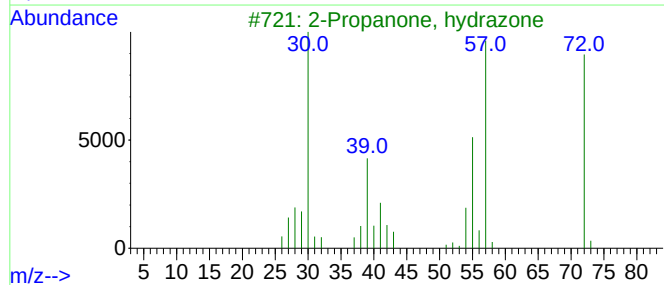
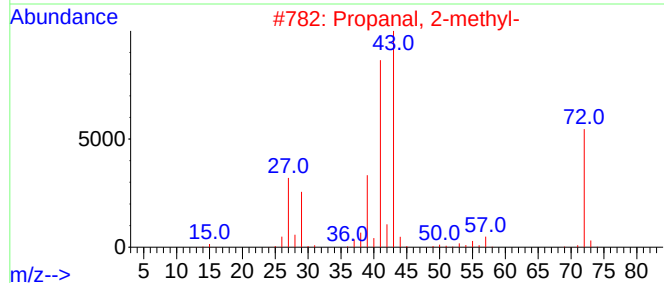
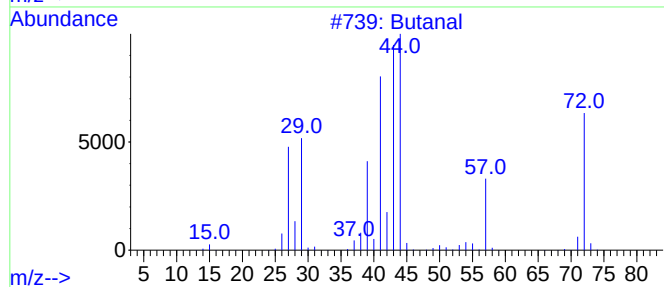
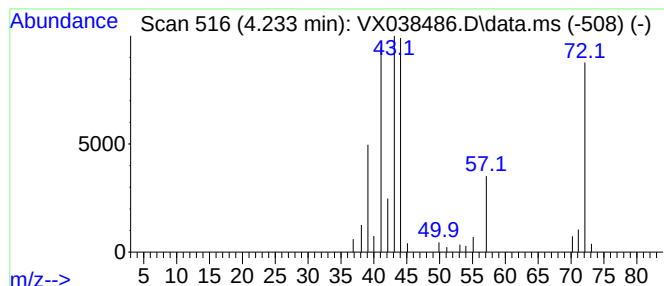
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	5.29 ug/l	50156	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
4			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	37
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37



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ALS Vial : 22 Sample Multiplier: 1

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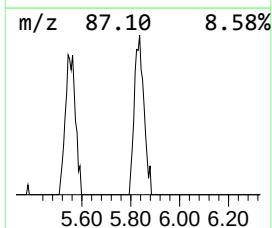
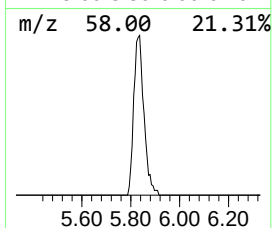
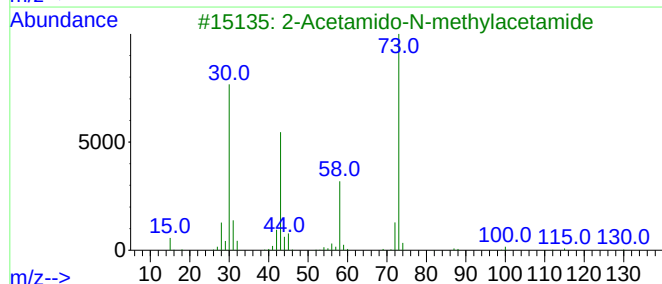
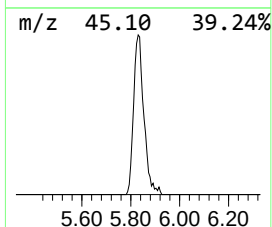
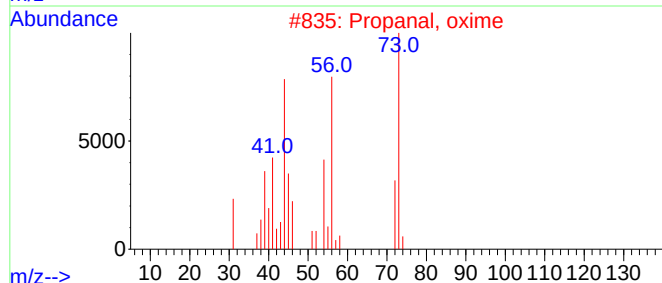
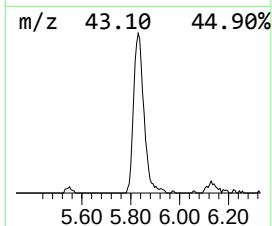
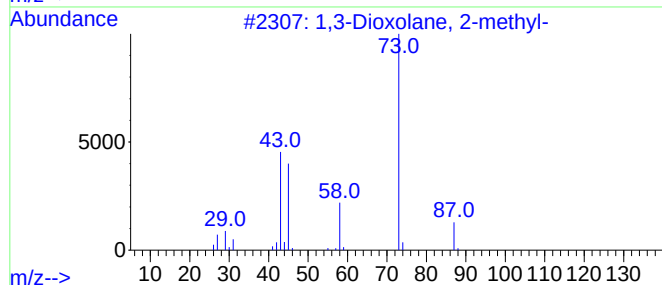
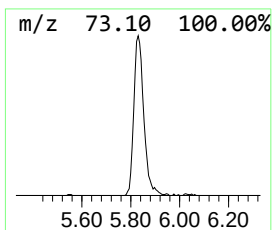
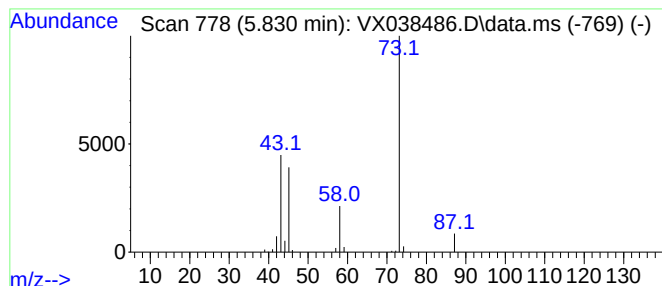
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

Peak Number 4 1,3-Dioxolane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.830	7.03 ug/l	66681	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	83		
2	Propanal, oxime	73	C3H7NO	000627-39-4	47		
3	2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	47		
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	28		
5	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9		



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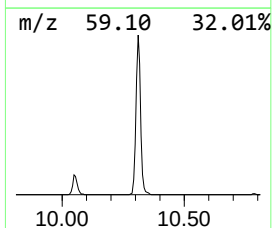
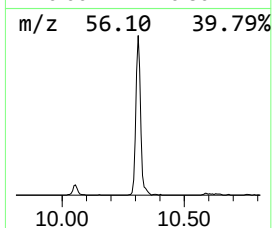
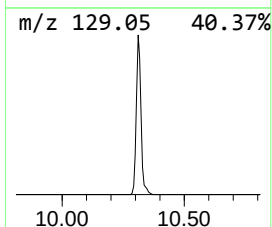
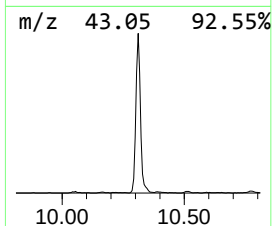
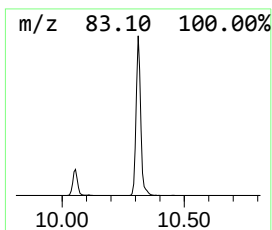
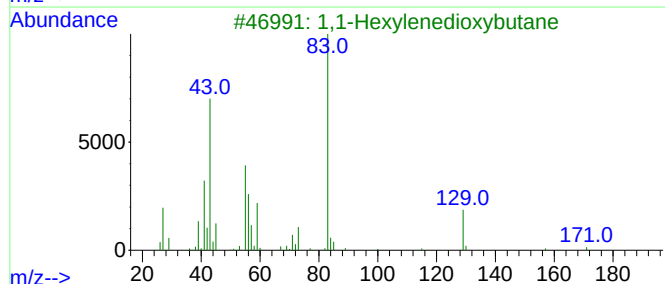
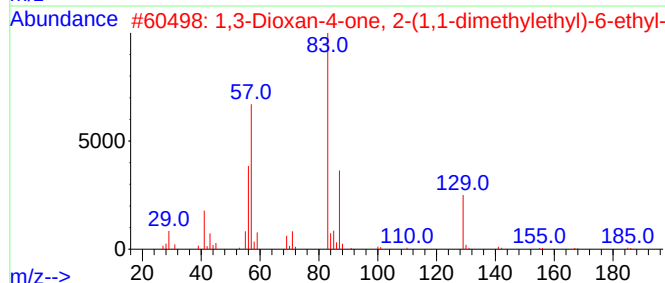
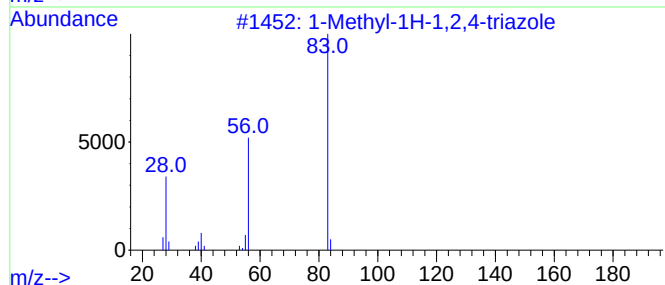
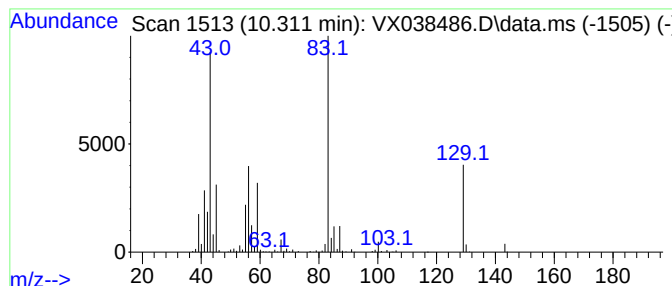
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown10.311 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.311	19.77 ug/l	344325	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	38
2			1,3-Dioxan-4-one, 2-(1,1-dimethy...	186	C10H18O3	113505-80-9	36
3			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	23
4			4H-1,2,4-Triazole, 4-methyl-	83	C3H5N3	010570-40-8	12
5			3-Methylbut-2-enoic acid, 3,4-di...	244	C11H10Cl2O2	1000307-59-7	10



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	232.7	ug/l	2207810	1	5.556	474497	50.0
Ethanol	2.050	6.5	ug/l	61623	1	5.556	474497	50.0
Butanal	4.233	5.3	ug/l	50156	1	5.556	474497	50.0
1,3-Dioxolane, ...	5.830	7.0	ug/l	66681	1	5.556	474497	50.0
unknown10.311	10.311	19.8	ug/l	344325	3	10.055	870780	50.0