

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051721\
 Data File : VN067106.D
 Acq On : 17 May 2021 17:00
 Operator : JC/MD
 Sample : M2388-12
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41769

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_N\methods\82N051421W.M

Title : SW846 8260

Signal : TIC: VN067106.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.297	193	208	243	rBV	2579018	4589417	3.23%	1.421%
2	3.638	667	708	744	rBV8	22213703	142168200	100.00%	44.013%
3	6.066	1547	1613	1691	rBV	9596256	53634112	37.73%	16.604%
4	7.597	2169	2184	2209	rVB	830578	1995100	1.40%	0.618%
5	8.525	2516	2530	2564	rVB	1269510	2732942	1.92%	0.846%
6	10.035	3075	3093	3108	rBV	1799018	3321208	2.34%	1.028%
7	10.298	3172	3191	3228	rVV	28071881	58921937	41.45%	18.241%
8	10.445	3229	3246	3292	rVB	22806425	44612695	31.38%	13.811%
9	11.357	3564	3586	3620	rBV2	1720799	4663095	3.28%	1.444%
10	12.320	3931	3945	3952	rBV	1329478	2205295	1.55%	0.683%
11	12.355	3952	3958	3996	rVB	1123912	2018675	1.42%	0.625%
12	13.296	4296	4309	4339	rBV	1188039	2149948	1.51%	0.666%

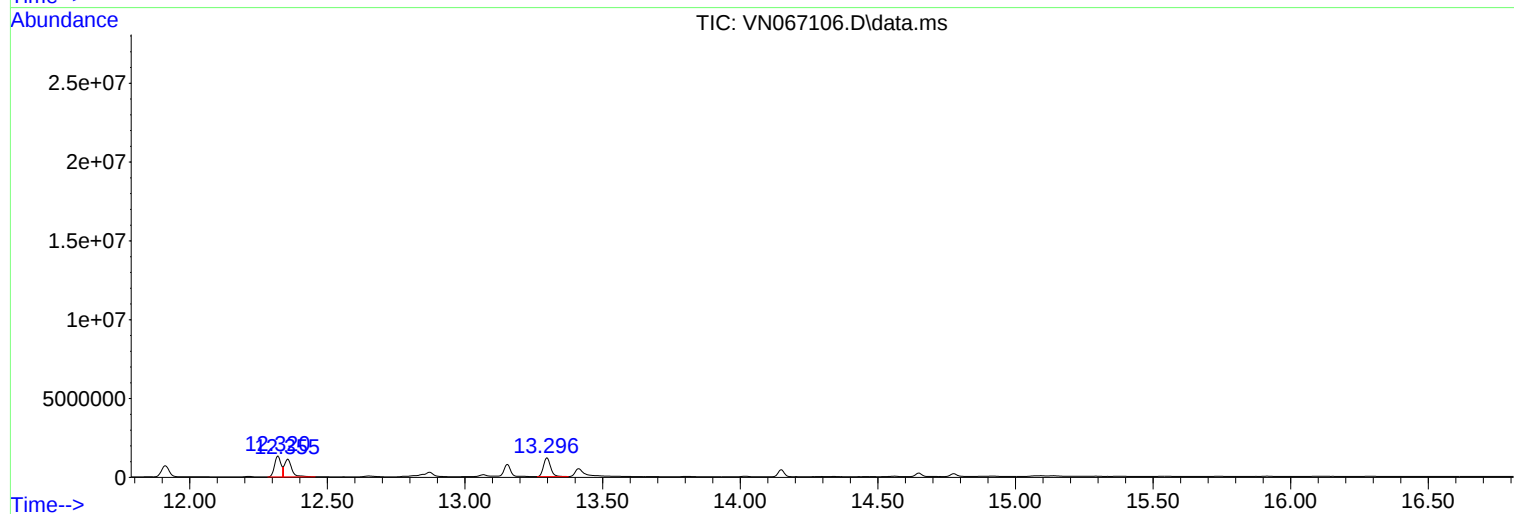
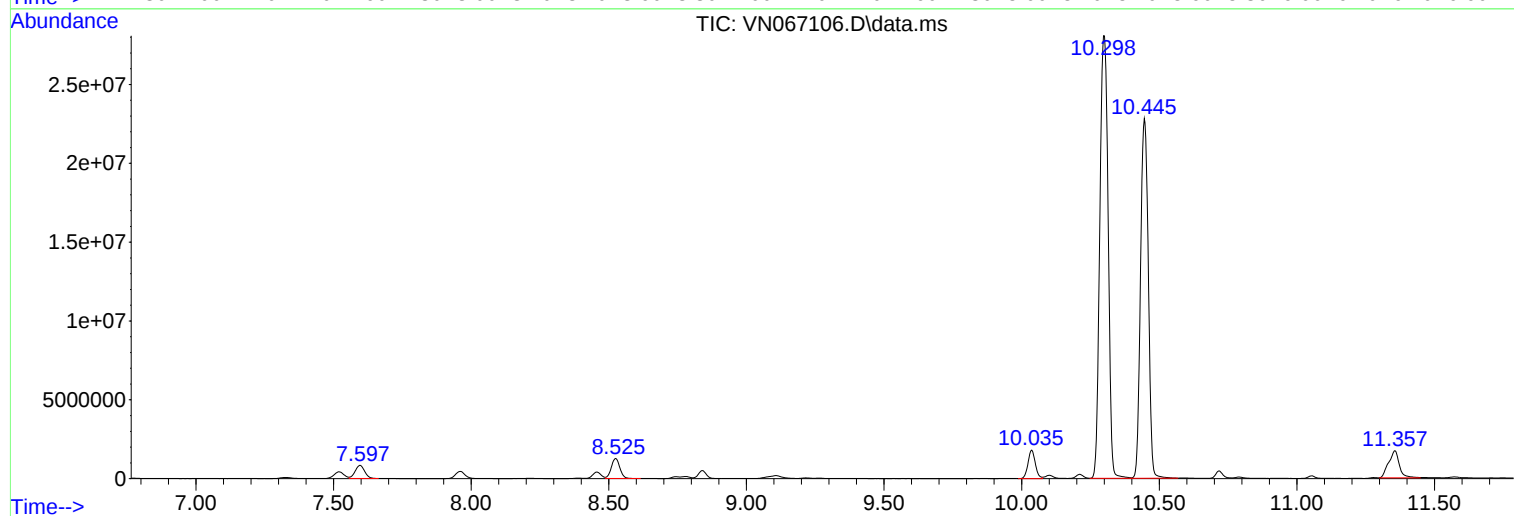
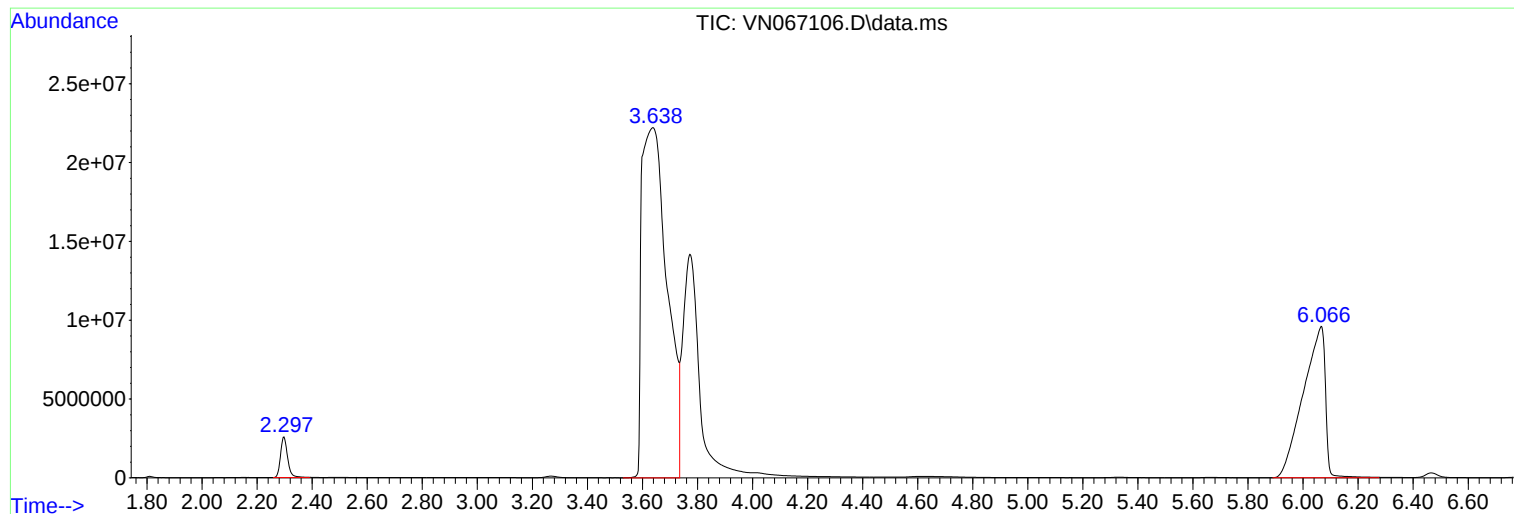
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

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



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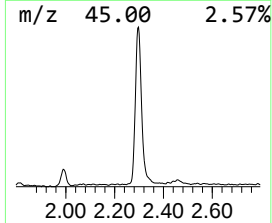
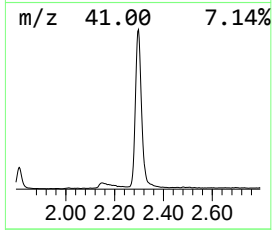
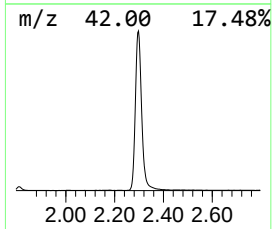
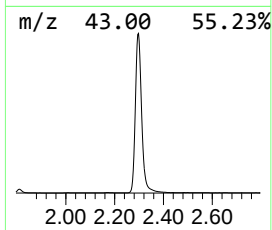
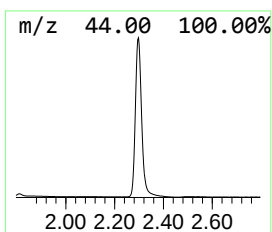
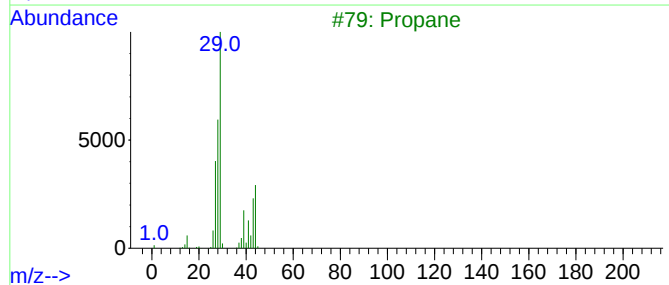
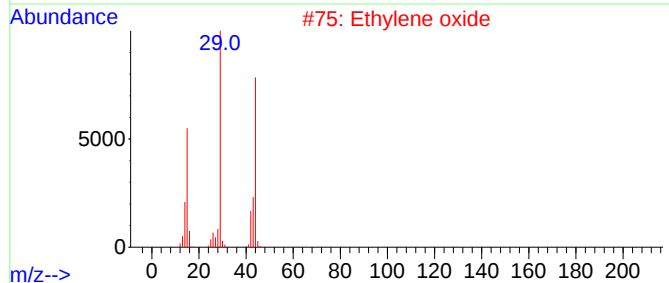
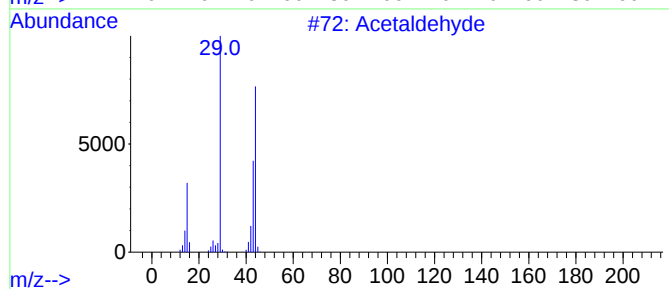
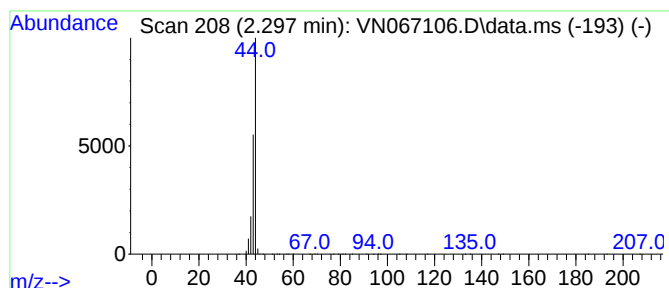
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.297	115.02 ug/l	4589420	Pentafluorobenzene	7.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Alanine	89	C3H7NO2	000056-41-7	4
5			1,2-Propanediamine	74	C3H10N2	000078-90-0	4



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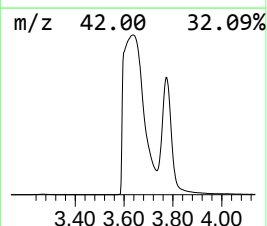
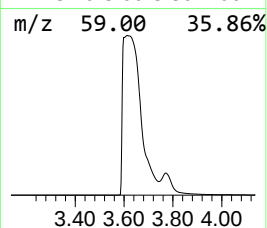
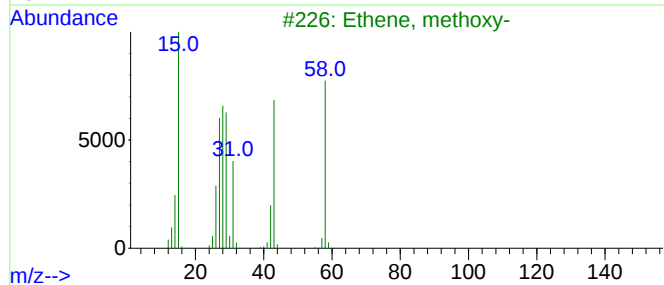
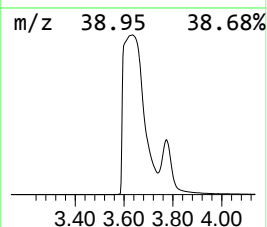
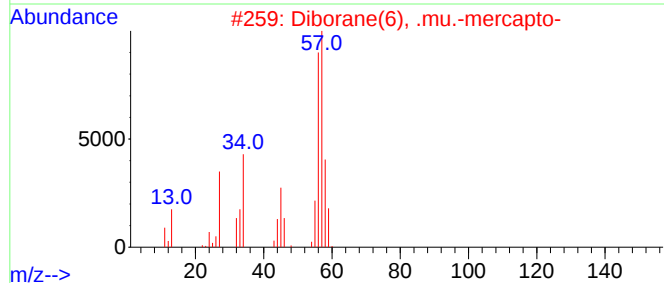
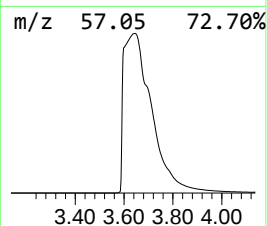
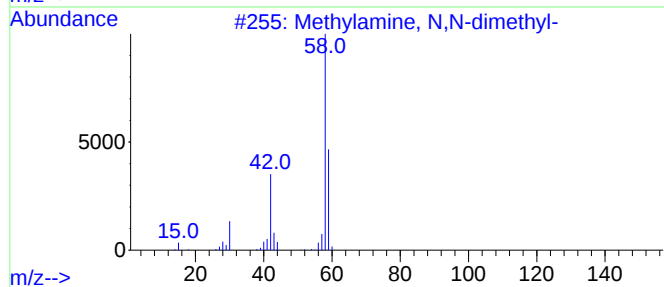
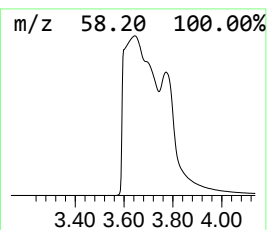
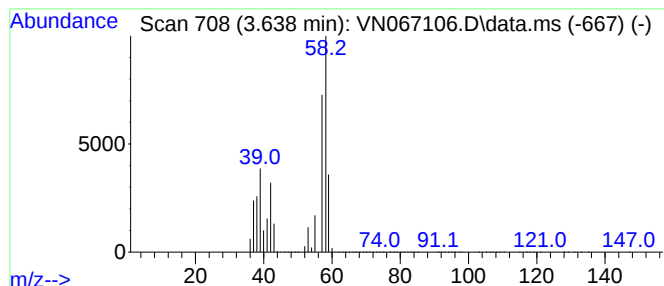
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown3.638 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.638	3562.93 ug/l	142168000	Pentafluorobenzene	7.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	22
2			Diborane(6), .mu.-mercapto-	60	B2H6S	022548-43-2	5
3			Ethene, methoxy-	58	C3H6O	000107-25-5	4
4			Propanal	58	C3H6O	000123-38-6	4
5			Diazene, dimethyl-	58	C2H6N2	000503-28-6	3



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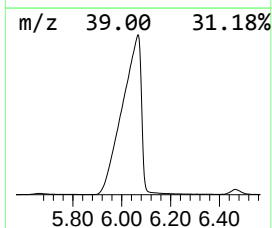
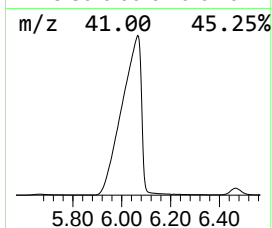
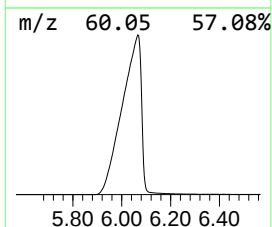
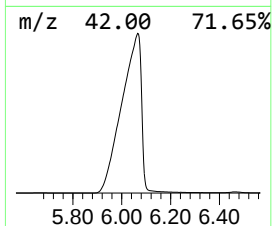
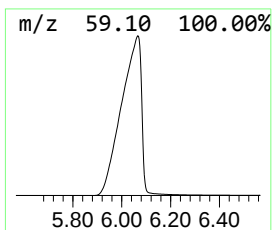
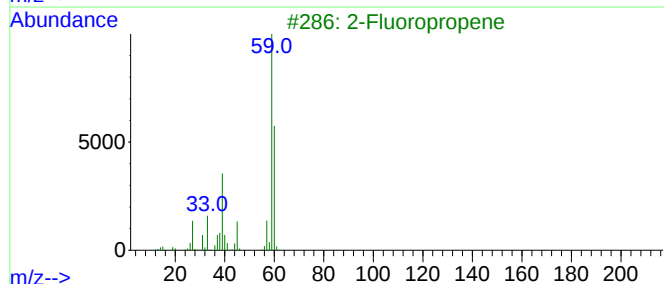
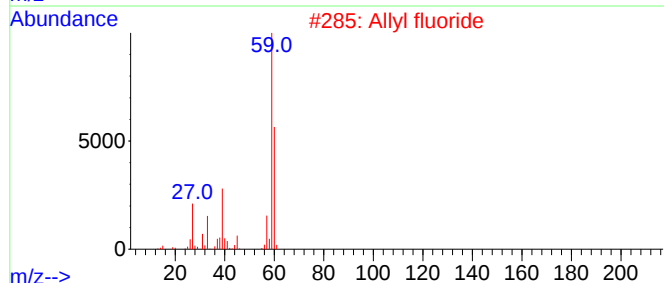
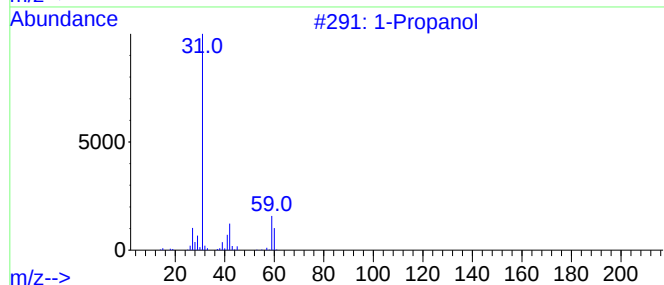
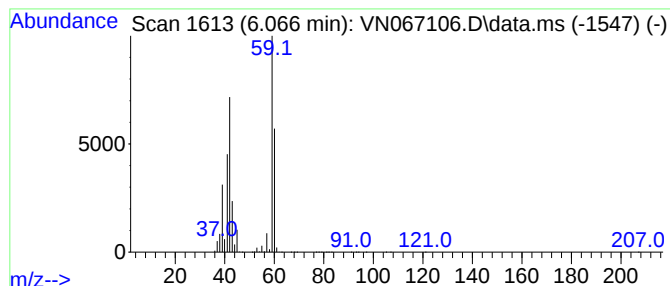
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.066	1344.15 ug/l	53634100	Pentafluorobenzene	7.597

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	78
2		Allyl fluoride	60	C3H5F	000818-92-8	53
3		2-Fluoropropene	60	C3H5F	001184-60-7	40
4		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9
5		Acetaldoxime	59	C2H5NO	000107-29-9	7



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ALS Vial : 18 Sample Multiplier: 1

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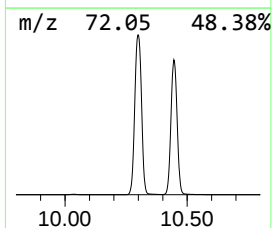
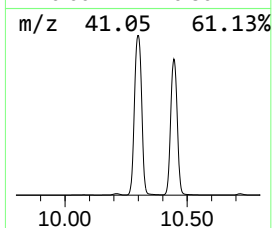
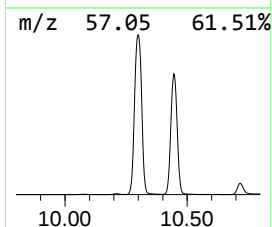
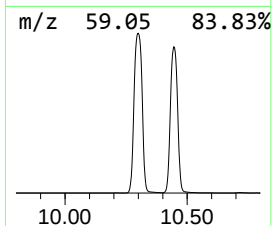
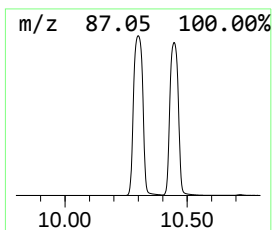
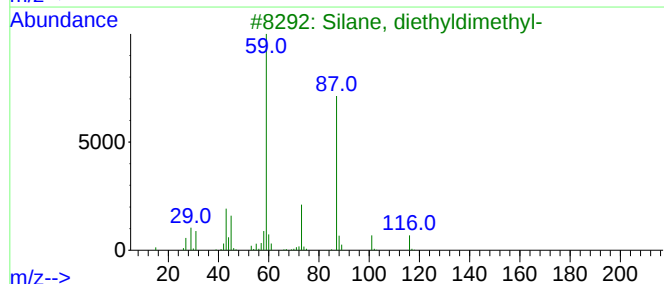
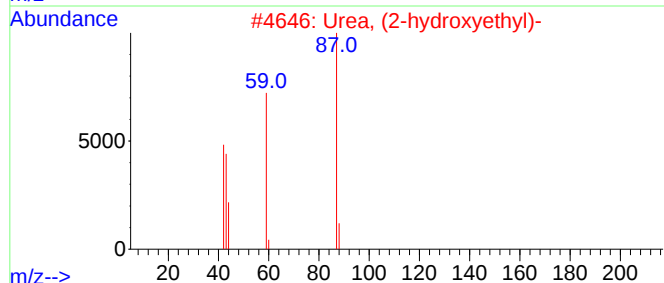
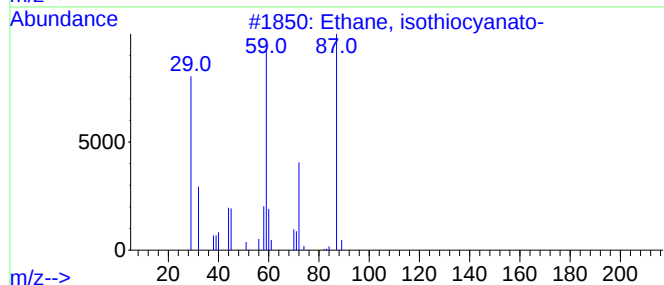
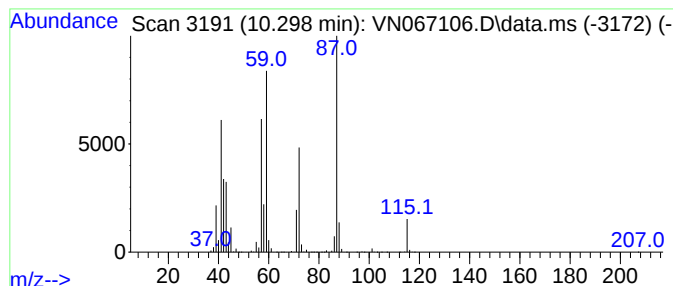
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Quant Title : SW846 8260

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

Peak Number 4 Ethane, isothiocyanato- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.298	631.79 ug/l	58921900	Chlorobenzene-d5	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	59
2			Urea, (2-hydroxyethyl)-	104	C3H8N2O2	002078-71-9	50
3			Silane, diethyldimethyl-	116	C6H16Si	000756-81-0	38
4			(Methylthio)-acetonitrile	87	C3H5NS	035120-10-6	32
5			Ethanol, 2-[2-(2-methoxyethoxy)e...	206	C9H18O5	003610-27-3	28



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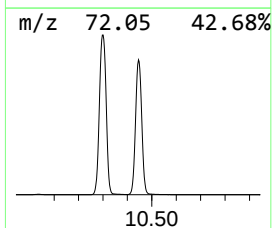
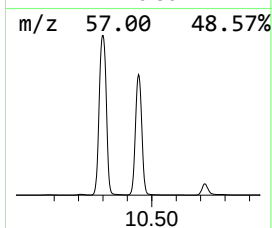
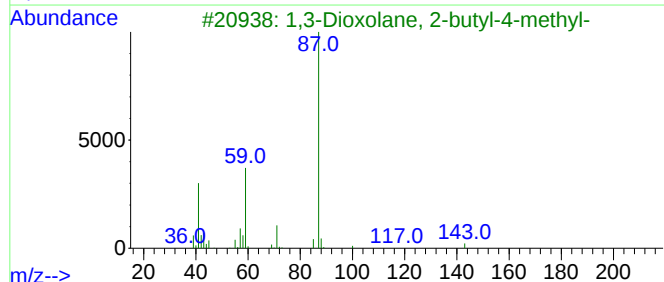
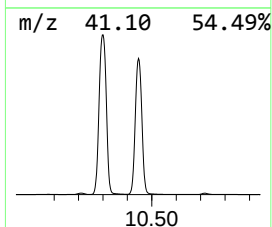
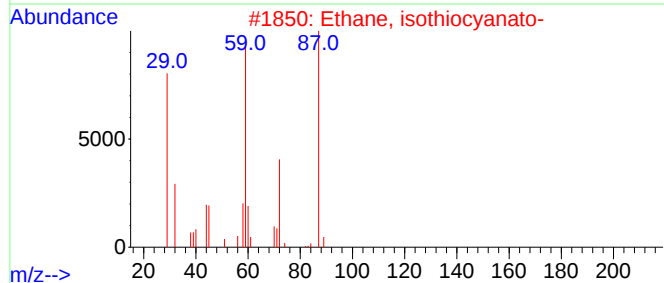
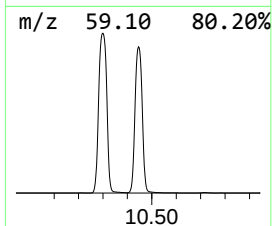
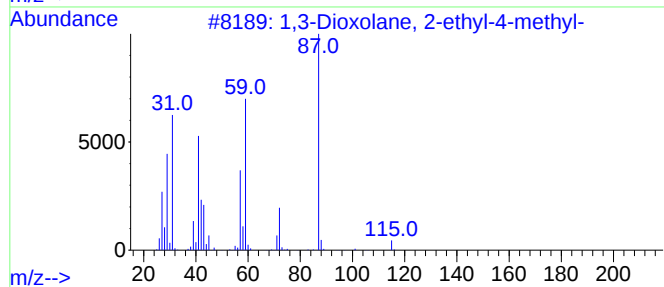
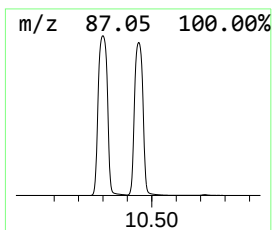
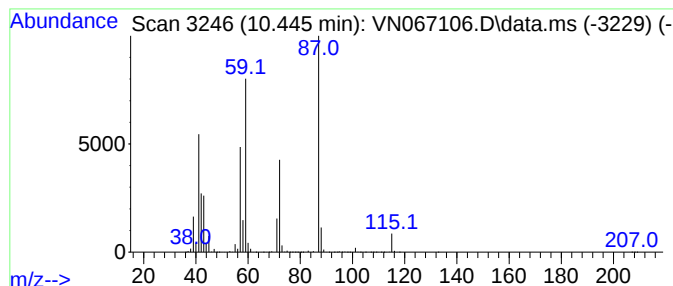
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Peak Number 5 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.445	478.36 ug/l	44612700	Chlorobenzene-d5	11.357	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	83
2	Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	64
3	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	59
4	Acetaldehyde, O-ethyl-oxime-	87	C4H9NO	1000288-34-6	45
5	Ethanol, 2-[2-(2-methoxyethoxy)e...	206	C9H18O5	003610-27-3	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.297	115.0	ug/l	4589420	1	7.597	1995100	50.0
unknown3.638	3.638	3562.9	ug/l	142168000	1	7.597	1995100	50.0
1-Propanol	6.066	1344.2	ug/l	53634100	1	7.597	1995100	50.0
Ethane, isothio...	10.298	631.8	ug/l	58921900	3	11.357	4663100	50.0
1,3-Dioxolane, ...	10.445	478.4	ug/l	44612700	3	11.357	4663100	50.0