

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
 Data File : VN070542.D
 Acq On : 10 Jan 2022 14:47
 Operator : JC/MD
 Sample : N1015-10 10X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31279

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\82N122721W.M

Title : SW846 8260

Signal : TIC: VN070542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.587	208	223	265	rVB	3828182	7072190	1.89%	0.975%
2	4.105	745	789	791	rBV3	70602471	77616079	20.71%	10.698%
3	6.627	1684	1729	1821	rBV	19355179	76734270	20.47%	10.576%
4	8.968	2586	2602	2641	rVB2	3169203	6839194	1.82%	0.943%
5	10.438	3128	3150	3162	rBV	3430702	6362496	1.70%	0.877%
6	10.502	3162	3174	3194	rVV	3836810	7138293	1.90%	0.984%
7	10.604	3194	3212	3225	rVV	3955145	7652702	2.04%	1.055%
8	10.692	3225	3245	3280	rVV7	151614288	374808405	100.00%	51.660%
9	10.829	3280	3296	3371	rVB4	71206237	130859492	34.91%	18.036%
10	11.706	3608	3623	3633	rBV	8008861	15642019	4.17%	2.156%
11	12.685	3969	3988	3997	rBV	6478651	10710263	2.86%	1.476%
12	13.672	4343	4356	4381	rVB2	2325581	4090703	1.09%	0.564%

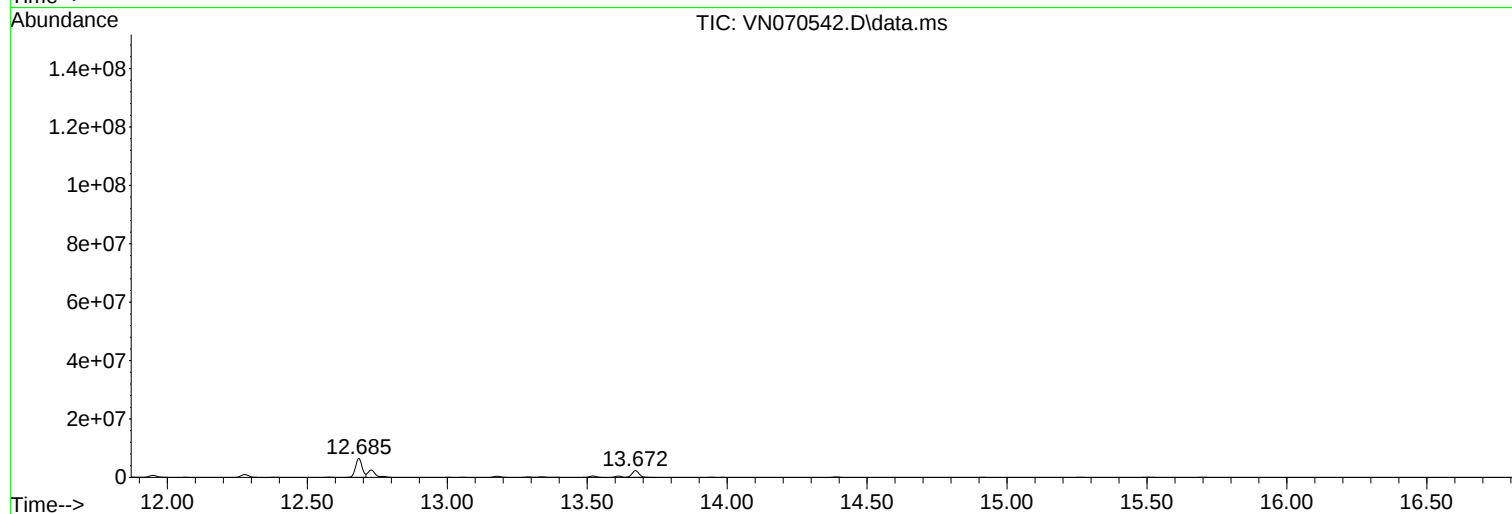
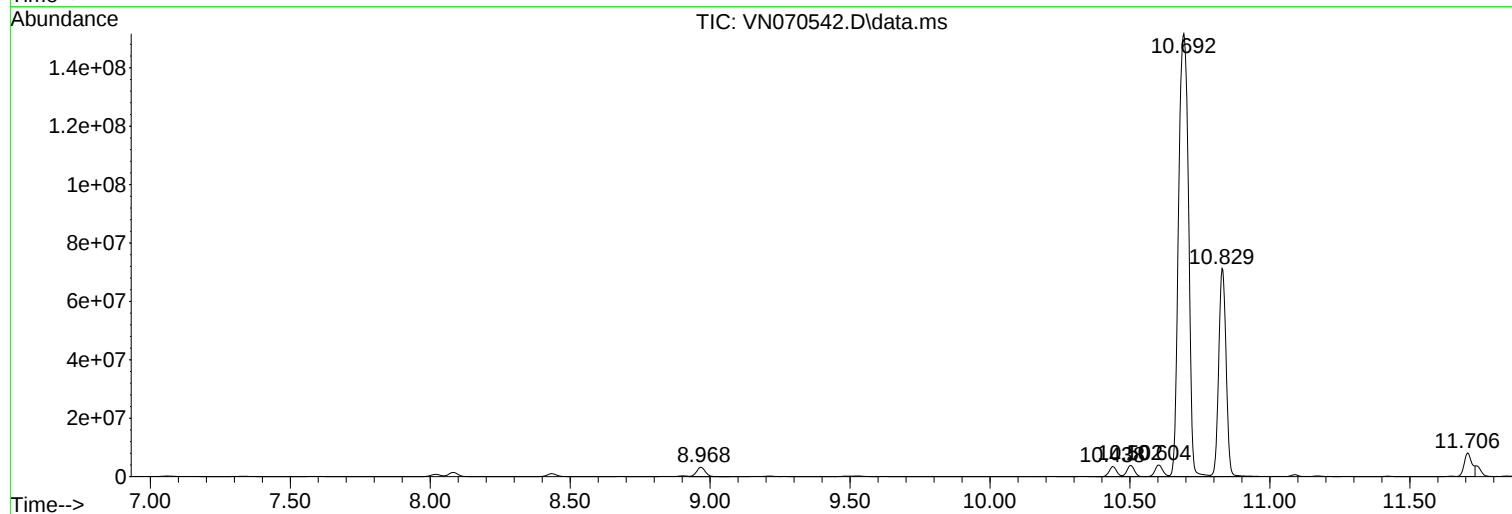
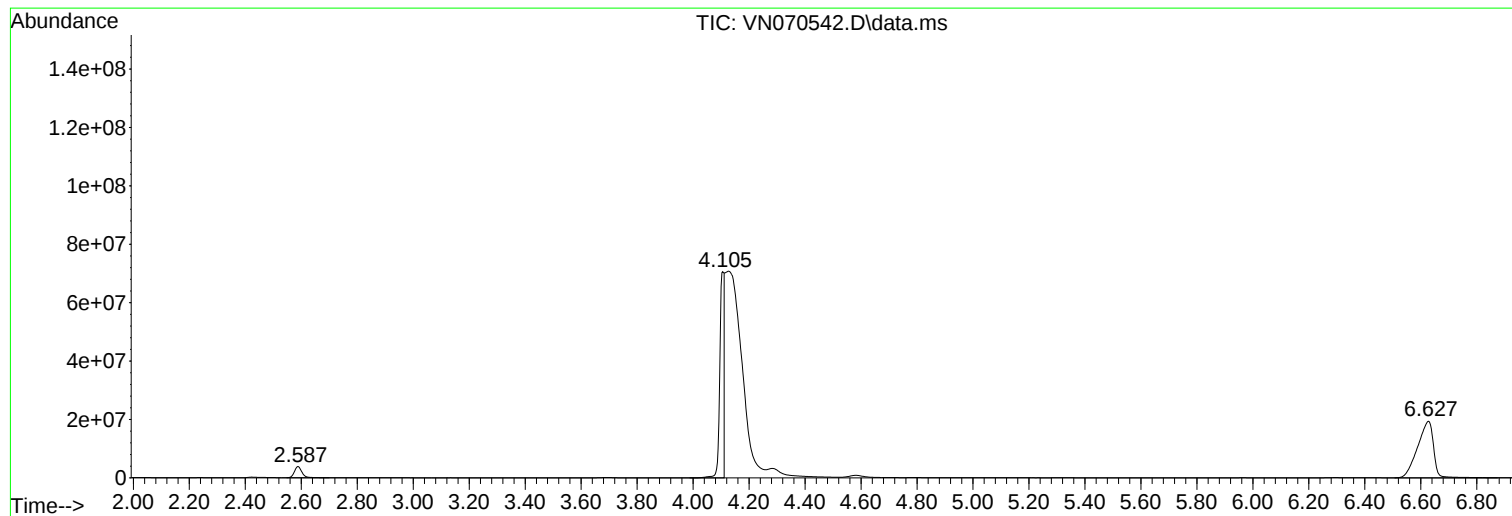
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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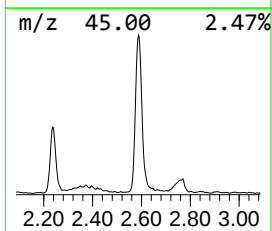
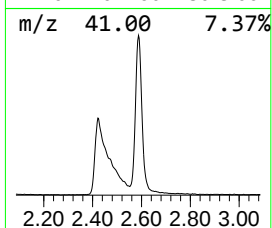
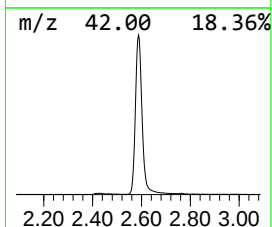
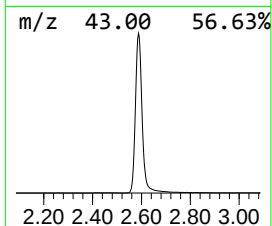
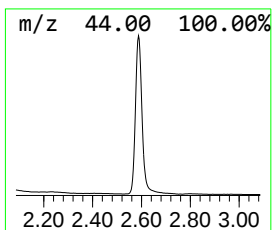
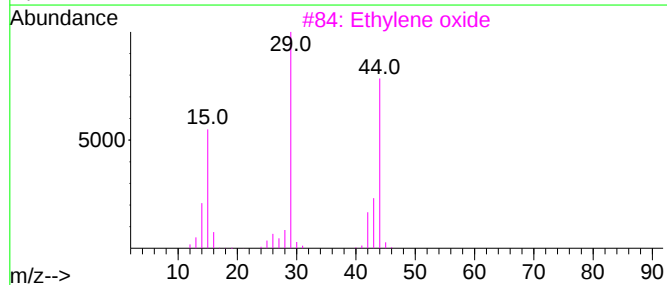
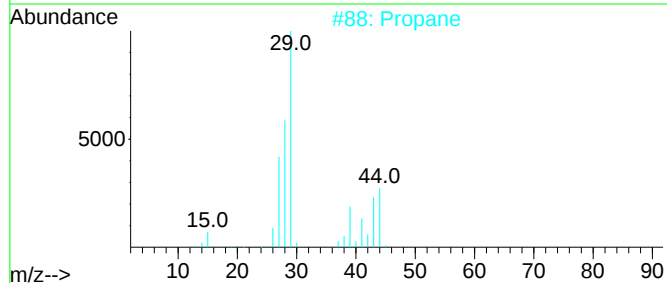
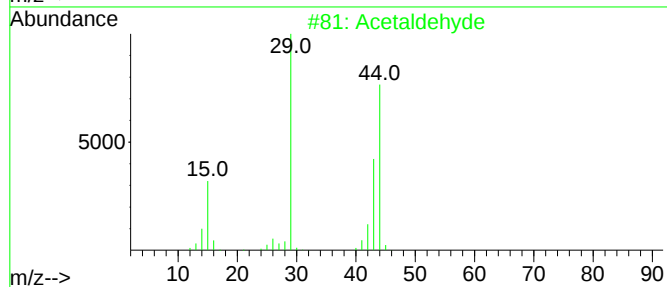
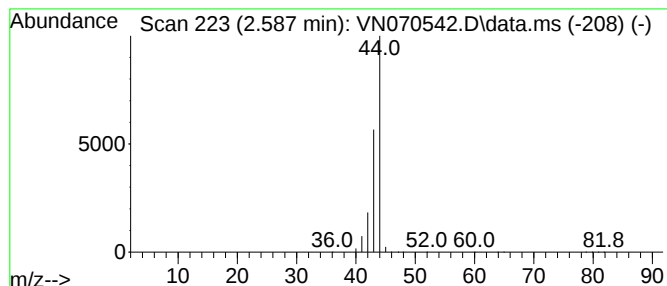
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.587 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.587	51.70 ug/l	7072190	Pentafluorobenzene	8.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	9
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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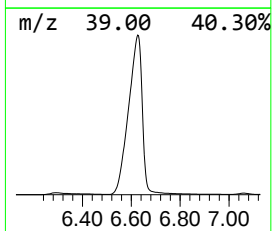
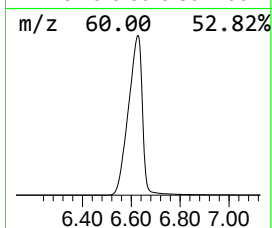
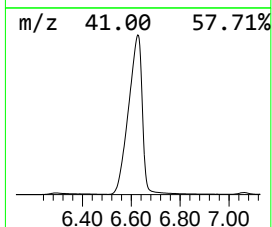
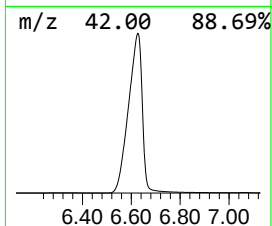
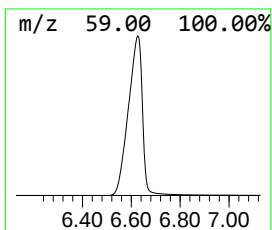
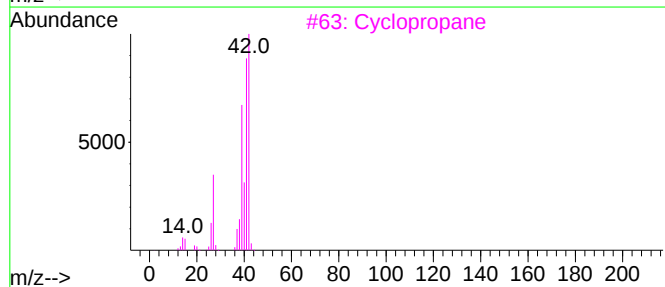
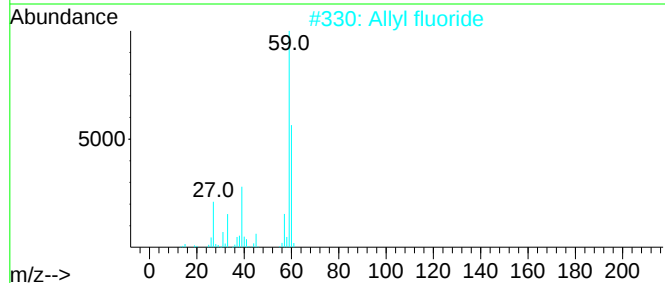
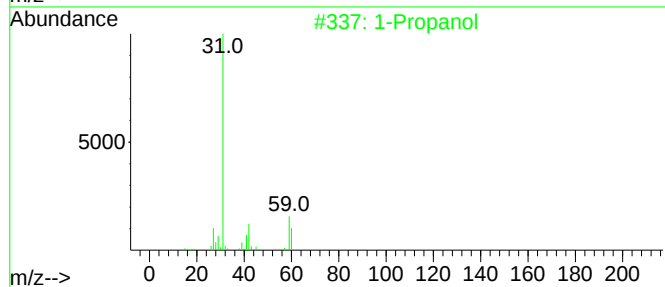
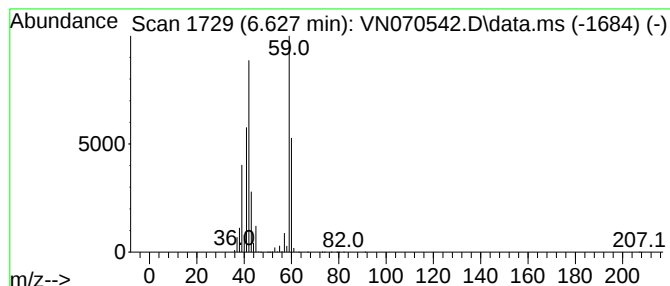
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.627	560.99 ug/l	76734300	Pentafluorobenzene	8.083

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	64
2		Allyl fluoride	60	C3H5F	000818-92-8	32
3		Cyclopropane	42	C3H6	000075-19-4	32
4		2-Fluoropropene	60	C3H5F	001184-60-7	27
5		Formamidoxime	60	CH4N2O	000624-82-8	9



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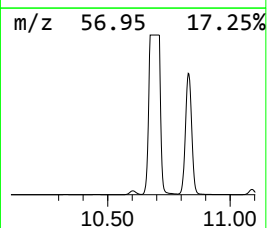
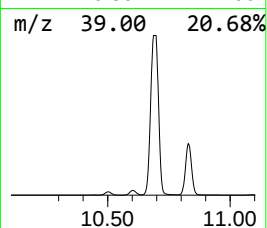
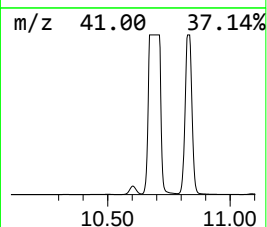
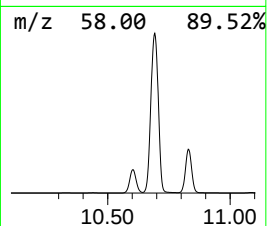
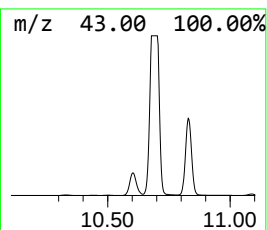
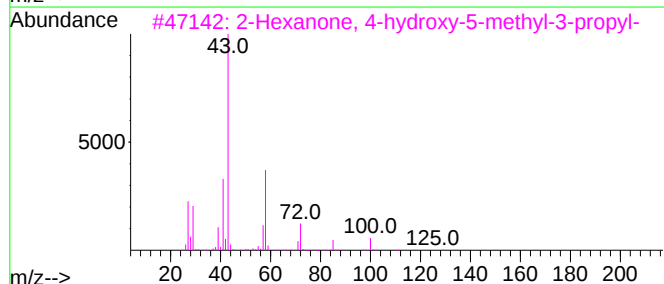
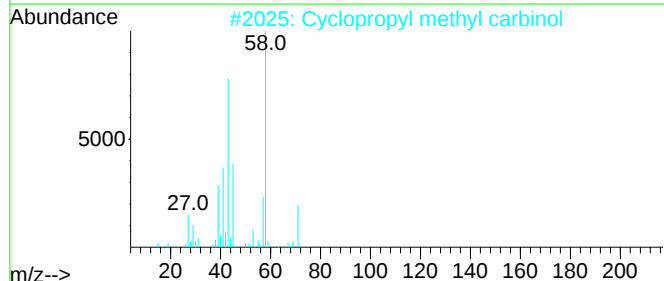
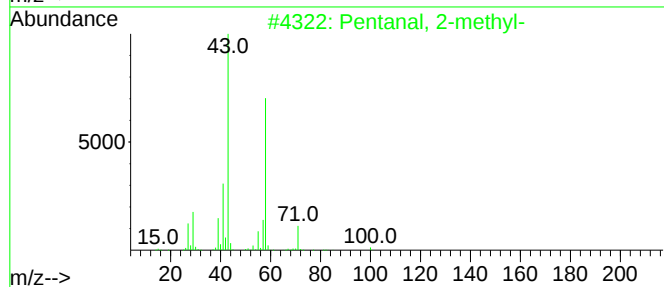
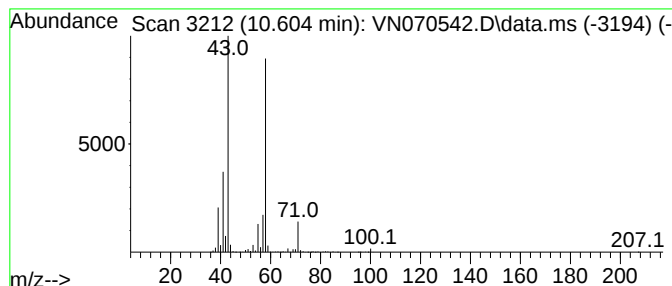
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentanal, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.604	24.46 ug/l	7652700	Chlorobenzene-d5	11.741

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	91
2			Cyclopropyl methyl carbinol	86	C5H10O	000765-42-4	56
3			2-Hexanone, 4-hydroxy-5-methyl-3...	172	C10H20O2	061141-74-0	40
4			Pentanal, 2,4-dimethyl-	114	C7H14O	027944-79-2	39
5			Phenylacetic acid, 2-dimethylami...	207	C12H17NO2	036882-00-5	38



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Sample : N1015-10 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

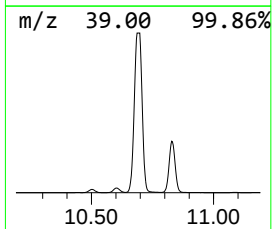
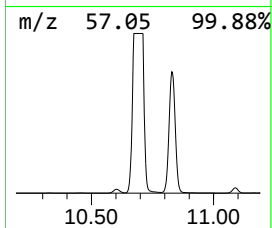
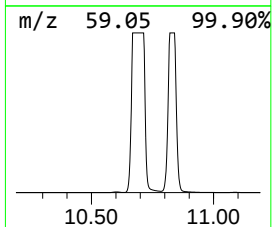
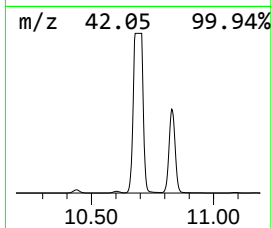
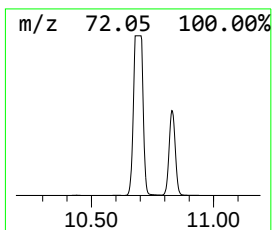
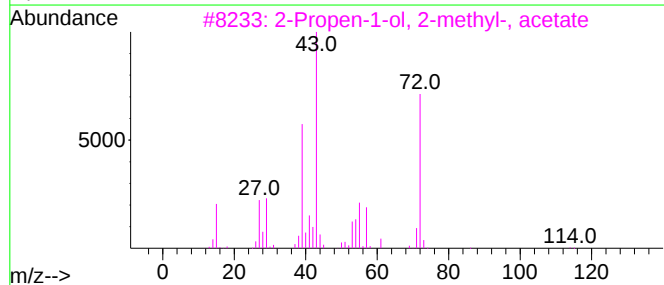
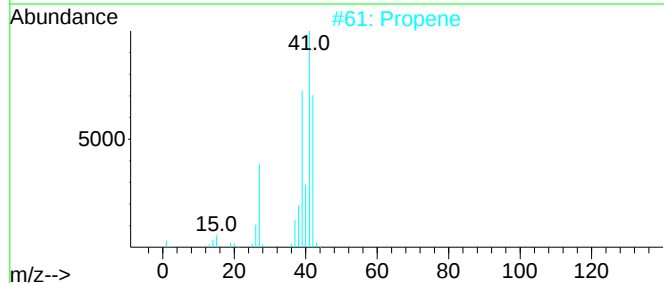
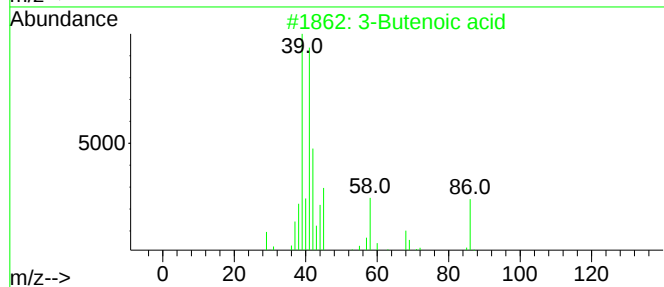
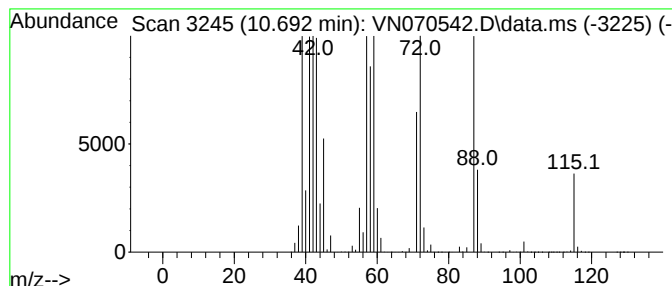
Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown10.692 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.692	1198.08 ug/l	374808000	Chlorobenzene-d5	11.741	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Butenoic acid	86	C4H6O2	000625-38-7	37
2	Propene	42	C3H6	000115-07-1	17
3	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	17
4	2-Butyn-1-ol, 4-methoxy-	100	C5H8O2	018857-03-9	17
5	2-Methyl-3-vinyl-oxirane	84	C5H8O	006790-37-0	16



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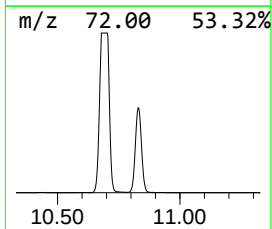
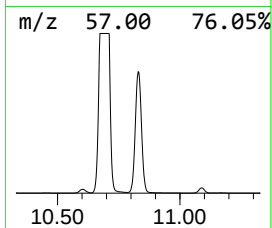
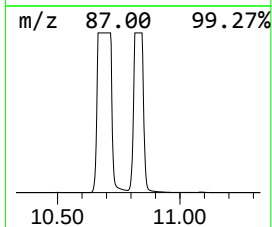
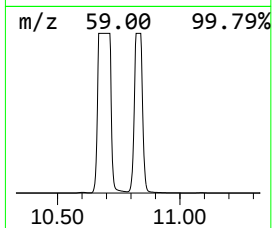
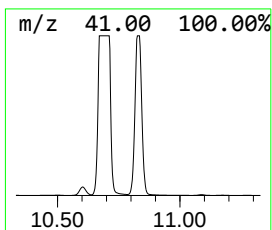
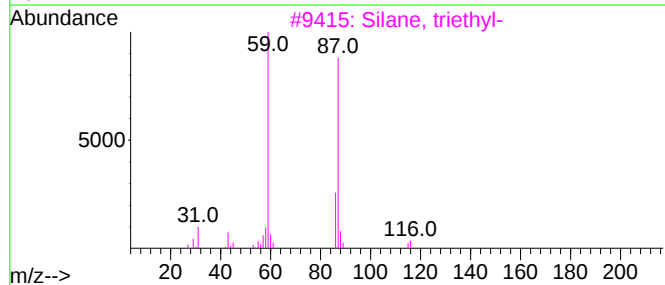
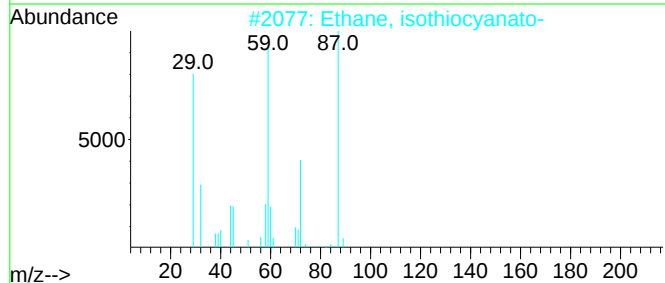
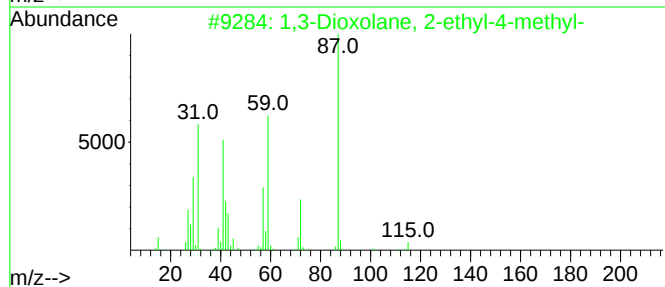
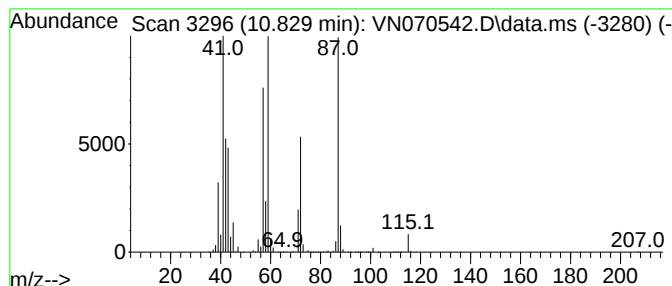
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.829	418.30 ug/l	130859000	Chlorobenzene-d5	11.741

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	53
2			Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	53
3			Silane, triethyl-	116	C6H16Si	000617-86-7	43
4			Urea, (2-hydroxyethyl)-	104	C3H8N2O2	002078-71-9	40
5			Propanamide, 2-methoxy-N-methyl-	117	C5H11NO2	1000196-12-6	38



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.587	2.587	51.7	ug/l	7072190	1	8.083	6839190	50.0
1-Propanol	6.627	561.0	ug/l	76734300	1	8.083	6839190	50.0
Pentanal, 2-met...	10.604	24.5	ug/l	7652700	3	11.741	15642000	50.0
unknown10.692	10.692	1198.1	ug/l	374808000	3	11.741	15642000	50.0
1,3-Dioxolane, ...	10.829	418.3	ug/l	130859000	3	11.741	15642000	50.0