

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121923\
 Data File : VN080514.D
 Acq On : 19 Dec 2023 12:48
 Operator : JC\MD
 Sample : 05886-01 50X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 AUD-1295

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\82N121223W.M
 Title : SW846 8260

Signal : TIC: VN080514.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.665	113	121	129	rBV	66234	119988	2.41%	0.653%
2	4.283	385	396	412	rBV	1723546	4977107	100.00%	27.100%
3	4.424	412	420	432	rVB2	35373	115007	2.31%	0.626%
4	4.700	458	467	484	rVB2	27768	89056	1.79%	0.485%
5	6.718	798	810	823	rBV	531990	1611947	32.39%	8.777%
6	8.165	1046	1056	1061	rBV	178421	428624	8.61%	2.334%
7	8.224	1061	1066	1078	rVB	309910	675825	13.58%	3.680%
8	8.577	1117	1126	1137	rVB	166638	370604	7.45%	2.018%
9	9.100	1205	1215	1224	rBV	481633	984459	19.78%	5.360%
10	9.653	1300	1309	1317	rVB4	25406	51133	1.03%	0.278%
11	10.565	1454	1464	1472	rBV	623338	1183655	23.78%	6.445%
12	10.800	1496	1504	1518	rBV	2135081	3633528	73.00%	19.784%
13	10.947	1521	1529	1538	rBV	433283	749147	15.05%	4.079%
14	11.823	1671	1678	1679	rBV2	36130	53317	1.07%	0.290%
15	11.865	1679	1685	1693	rVB	728536	1268891	25.49%	6.909%
16	12.847	1846	1852	1862	rVB	517718	884607	17.77%	4.817%
17	13.794	2006	2013	2021	rVB	699824	1168947	23.49%	6.365%

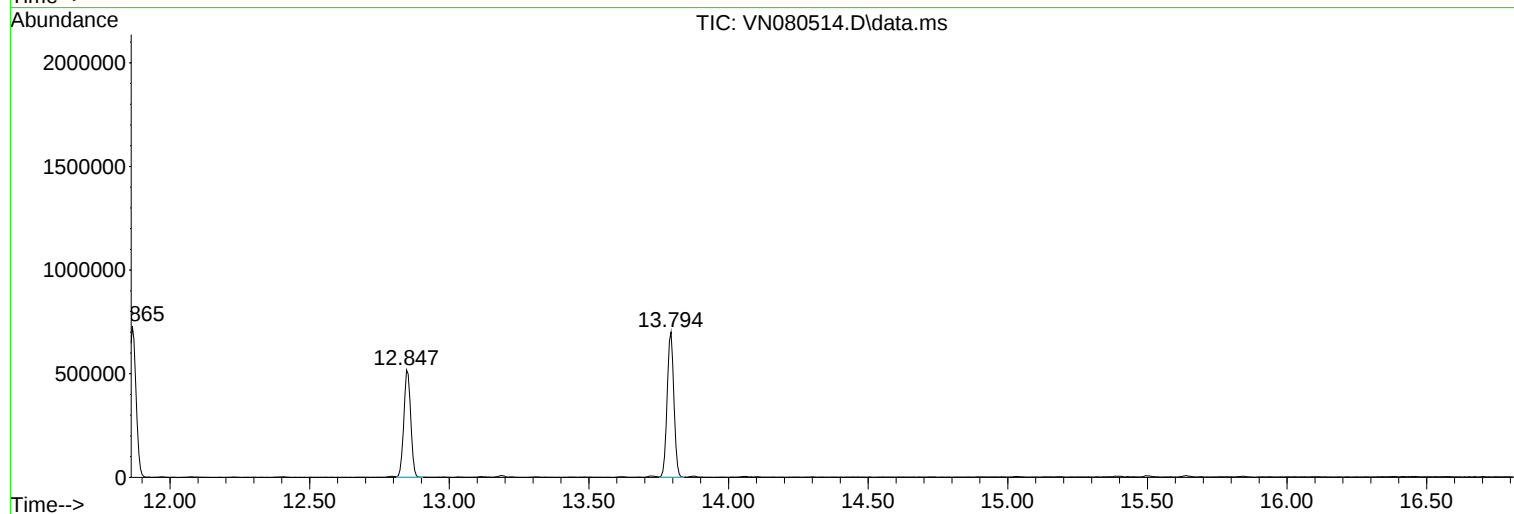
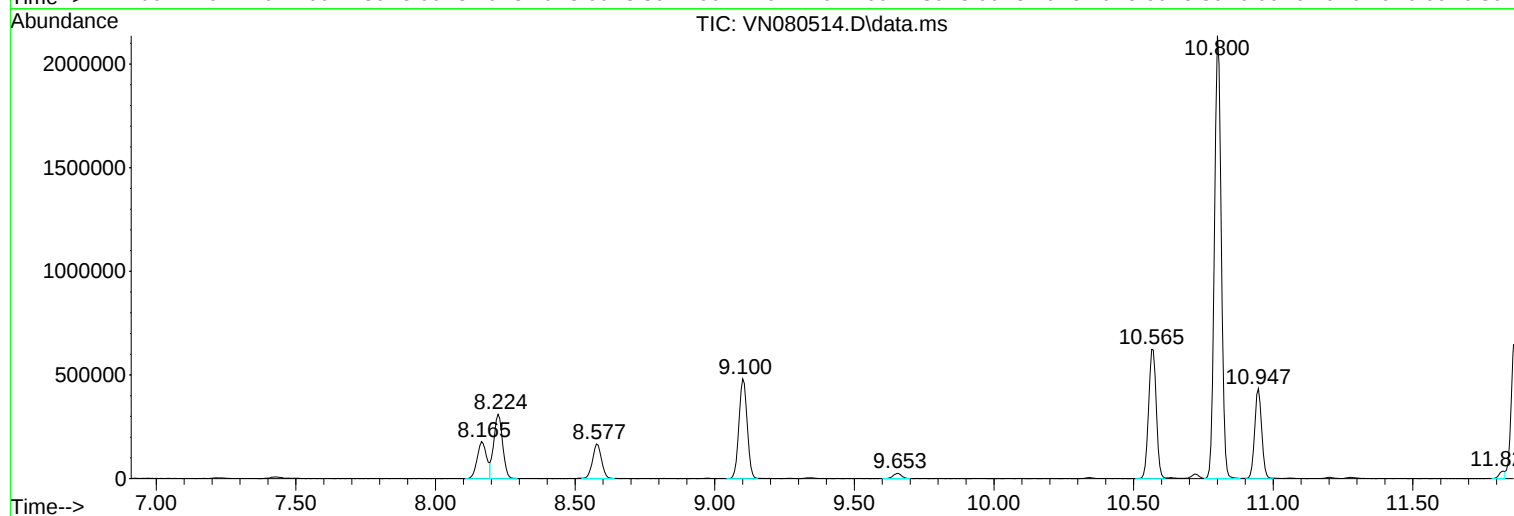
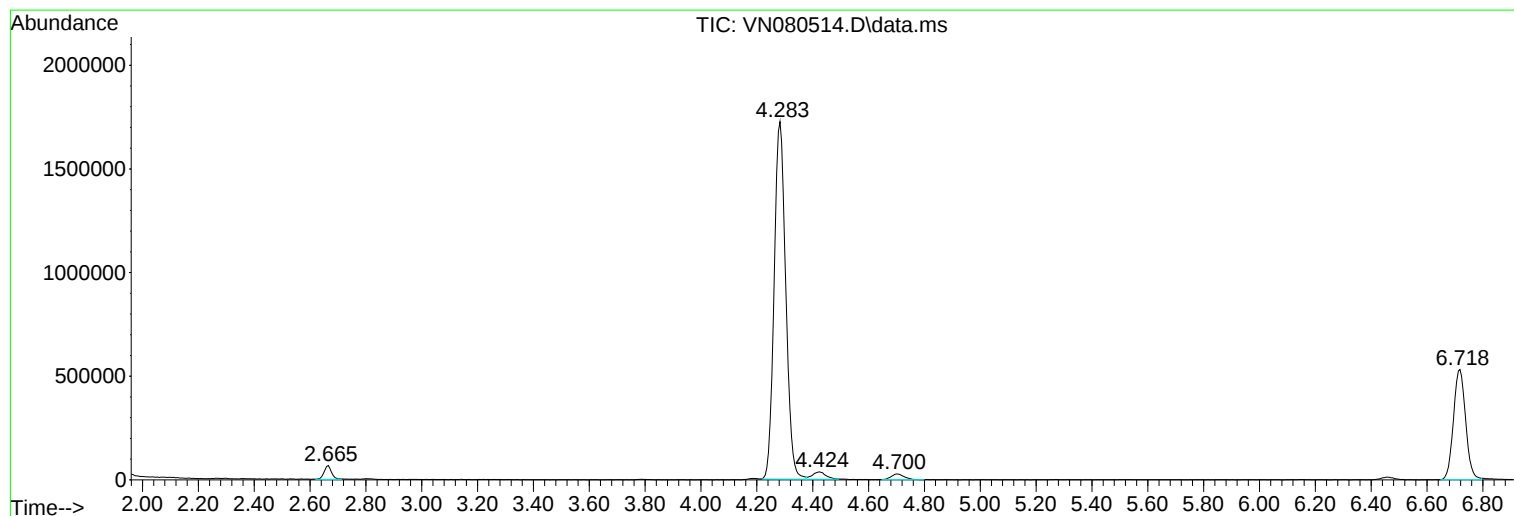
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Quant Title : SW846 8260

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



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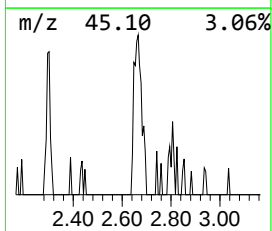
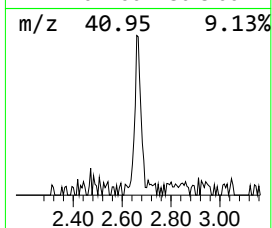
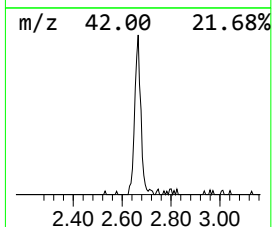
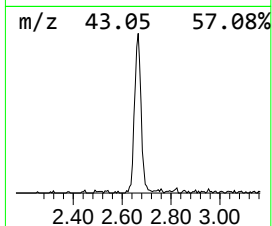
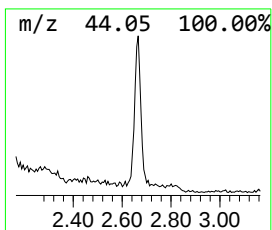
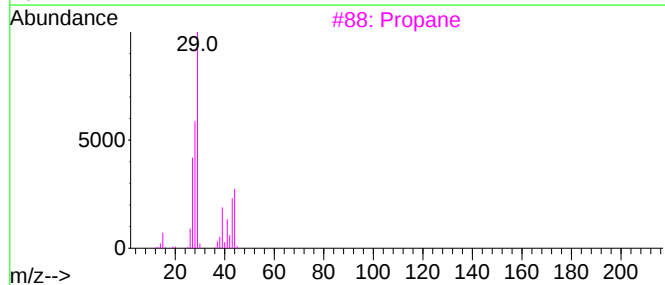
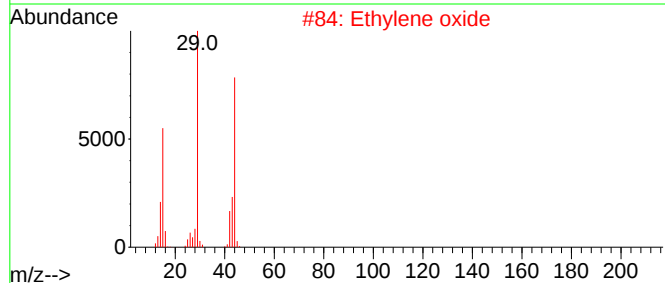
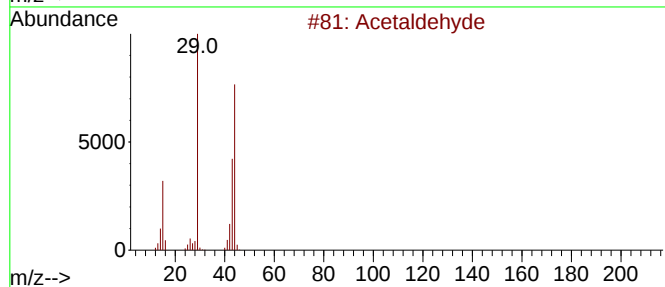
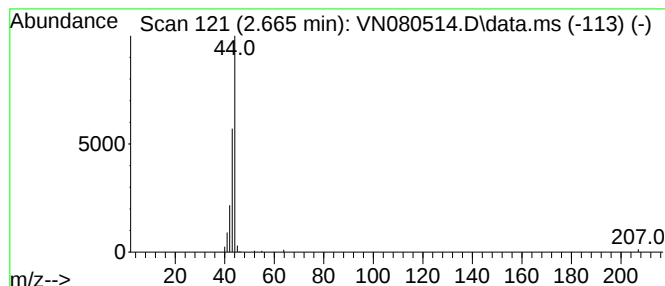
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Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.665	8.88 ug/l	119988	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
2			Ethylene oxide	44	C2H4O	000075-21-8	9
3			Propane	44	C3H8	000074-98-6	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			1-Propanol, 2-amino-, (+/-)-	75	C3H9NO	006168-72-5	4



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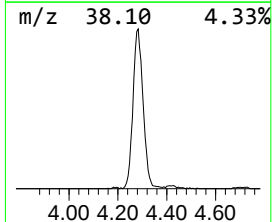
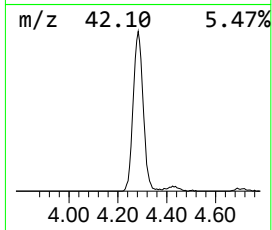
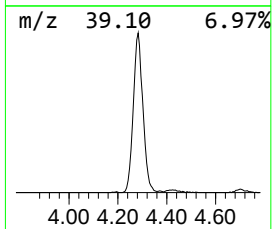
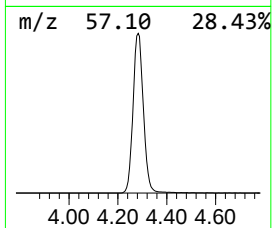
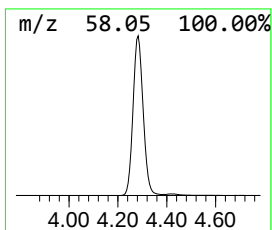
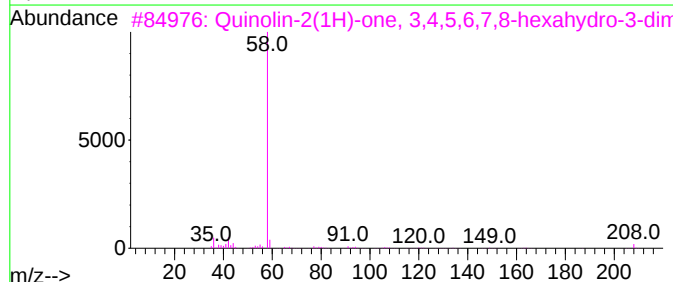
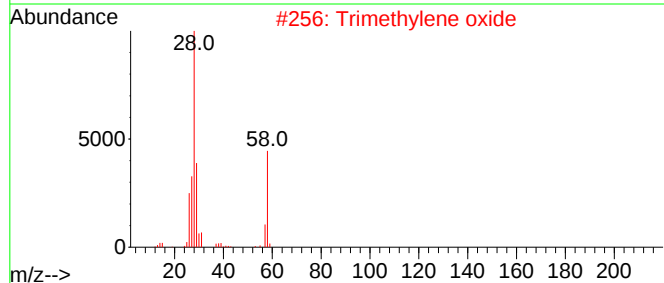
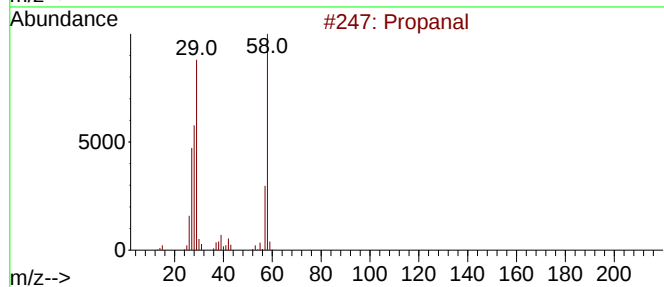
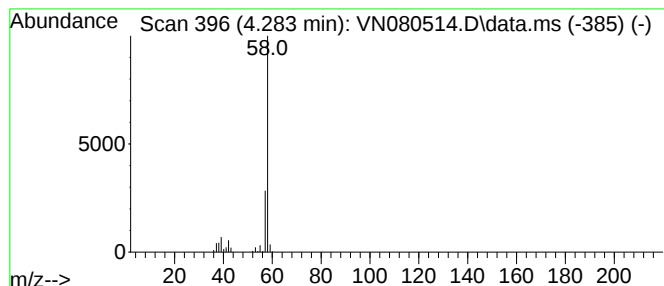
Instrument :
MSVOA_N
ClientSampleId :
AUD-1295

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.283	368.23 ug/l	4977110	Pentafluorobenzene	8.224	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	56
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4	Propylene oxide	58	C3H6O	000075-56-9	7
5	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	5



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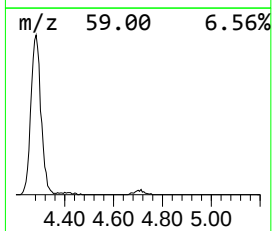
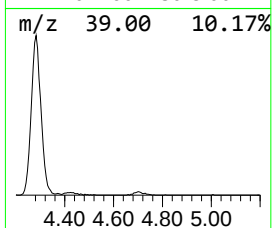
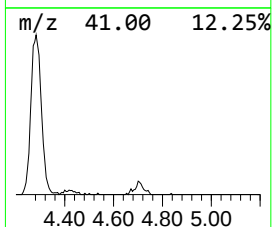
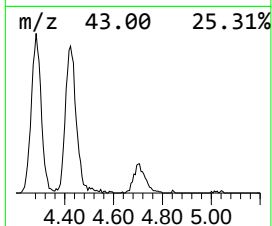
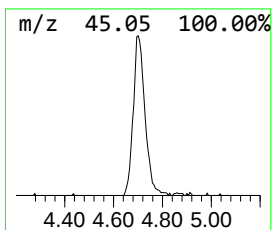
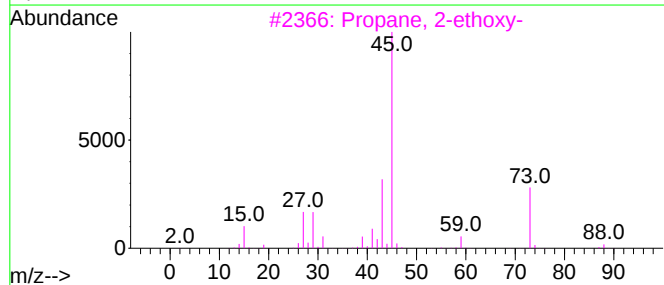
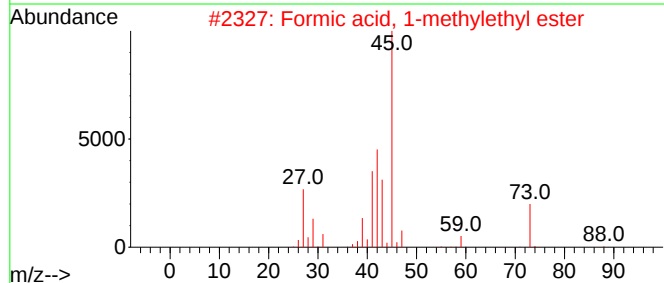
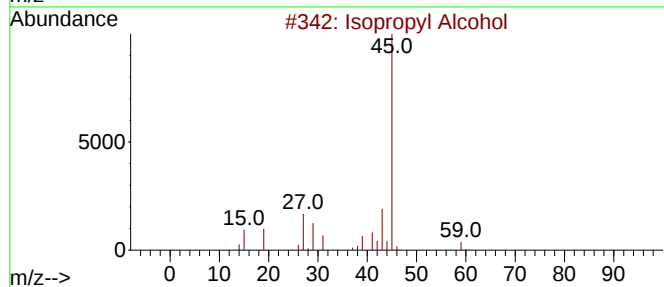
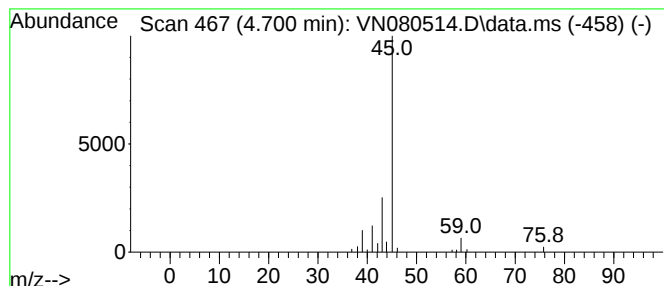
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.700	6.59 ug/l	89056	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
3			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
4			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
5			(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	9



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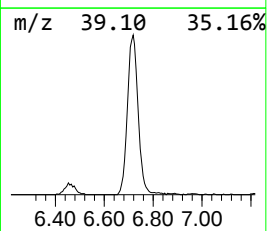
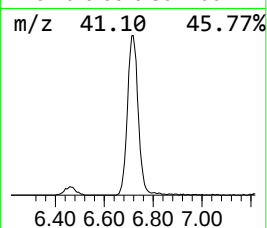
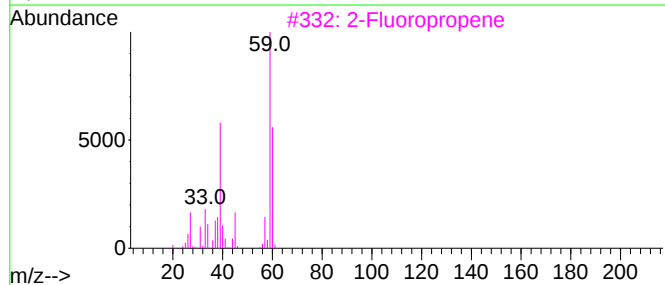
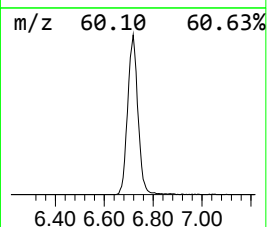
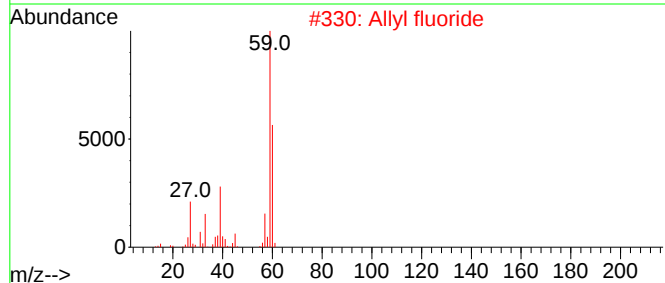
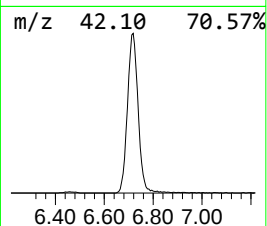
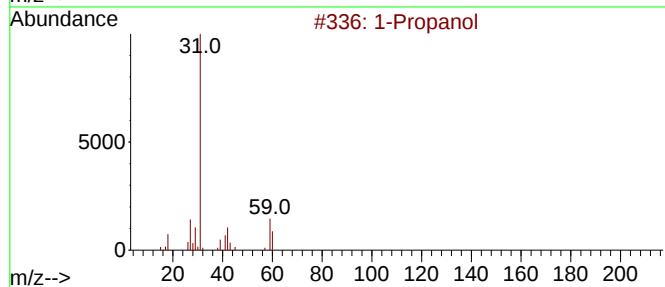
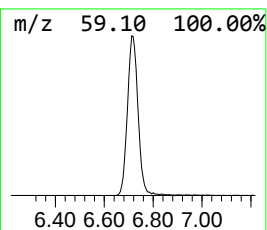
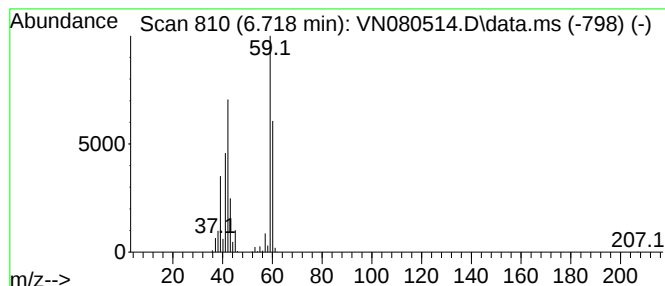
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.718	119.26 ug/l	1611950	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	72
2			Allyl fluoride	60	C3H5F	000818-92-8	58
3			2-Fluoropropene	60	C3H5F	001184-60-7	50
4			HEX-5-EN-3-OL	100	C6H12O	000688-99-3	23
5			Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	17



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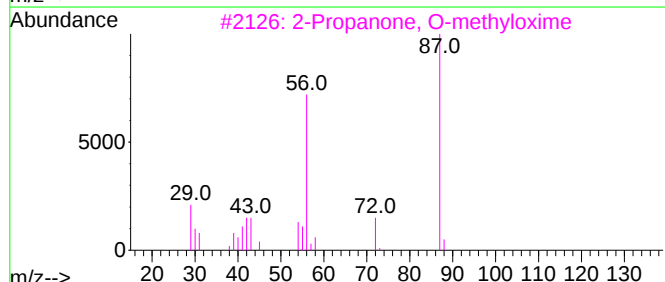
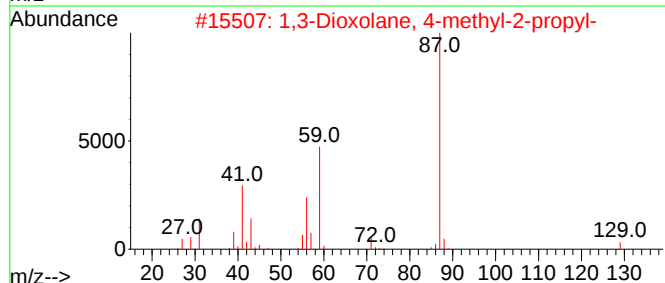
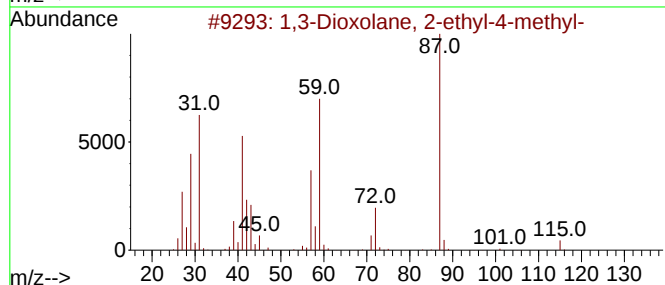
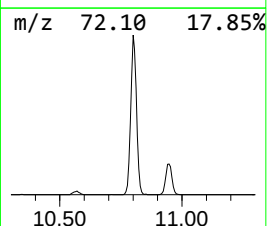
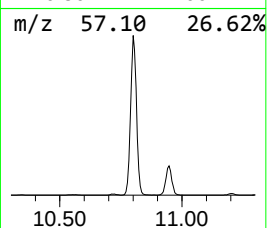
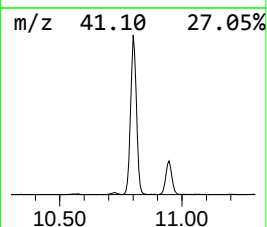
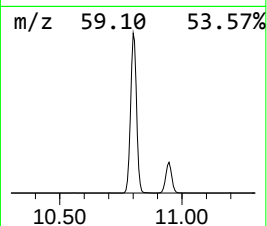
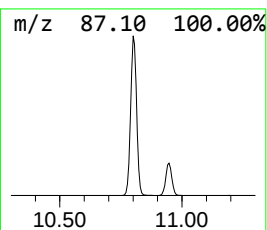
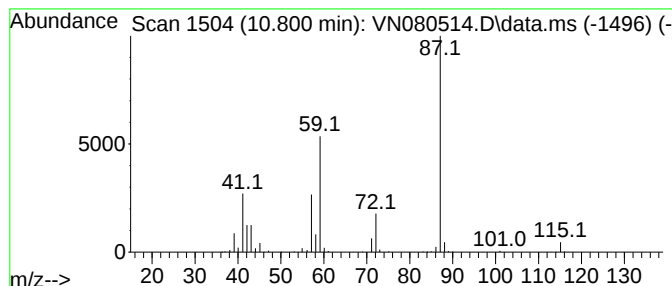
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.800	143.18 ug/l	3633530	Chlorobenzene-d5		11.865	
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	72
3	2-Propanone, O-methyloxime		87	C4H9NO	003376-35-0	52
4	Thiocyanic acid, ethyl ester		87	C3H5NS	000542-90-5	50
5	Acetamide, N-ethyl-		87	C4H9NO	000625-50-3	50



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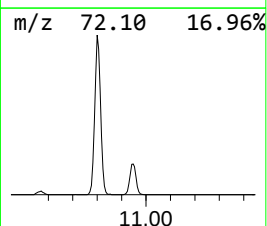
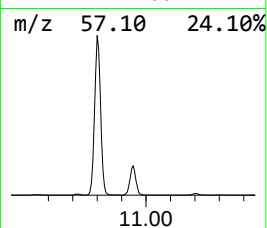
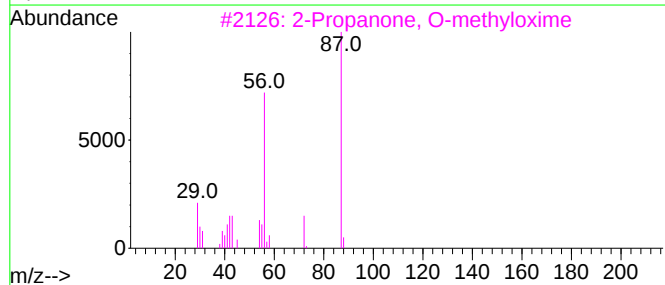
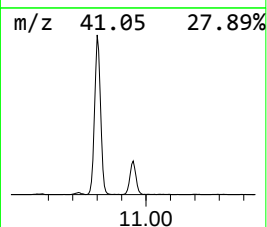
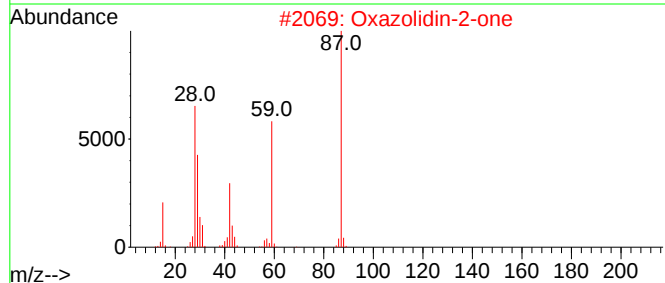
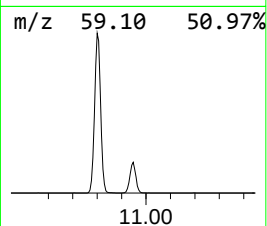
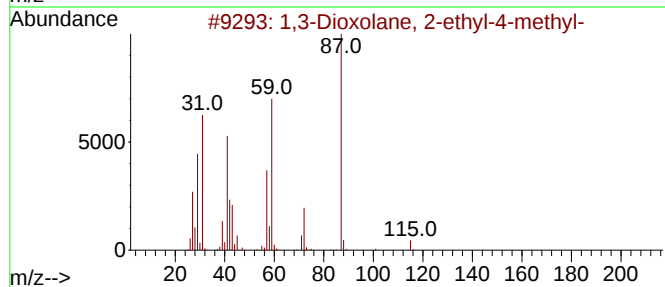
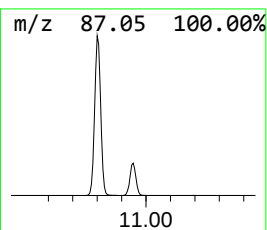
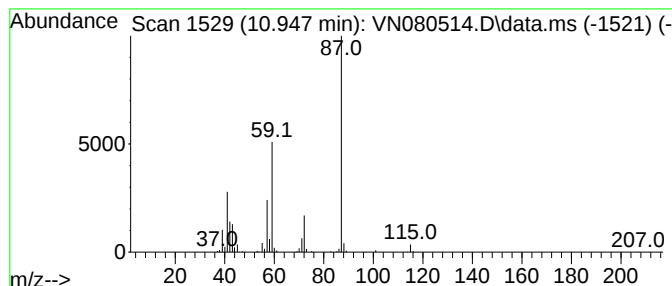
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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

Peak Number 6 Oxazolidin-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	29.52 ug/l	749147	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	80
3			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
4			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	50
5			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121923\
Data File : VN080514.D
Acq On : 19 Dec 2023 12:48
Operator : JC\MD
Sample : 05886-01 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1295

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.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
Acetaldehyde	2.665	8.9	ug/l	119988	1	8.224	675825	50.0
Propanal	4.283	368.2	ug/l	4977110	1	8.224	675825	50.0
Isopropyl Alcohol	4.700	6.6	ug/l	89056	1	8.224	675825	50.0
1-Propanol	6.718	119.3	ug/l	1611950	1	8.224	675825	50.0
1,3-Dioxolane, ...	10.800	143.2	ug/l	3633530	3	11.865	1268890	50.0
Oxazolidin-2-one	10.947	29.5	ug/l	749147	3	11.865	1268890	50.0