

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071923\
 Data File : VN078578.D
 Acq On : 19 Jul 2023 14:12
 Operator : JC\MD
 Sample : 03664-05 200X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 AUD-1012

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\82N071023W.M
 Title : SW846 8260

Signal : TIC: VN078578.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.306	53	60	68	rBV	165642	262208	10.82%	1.235%
2	2.671	116	122	134	rBV	590177	1005196	41.48%	4.734%
3	2.824	142	148	155	rVB3	22069	45434	1.87%	0.214%
4	4.300	386	399	414	rBV	446295	1270692	52.44%	5.984%
5	4.442	414	423	444	rVB	235880	694697	28.67%	3.271%
6	4.730	460	472	487	rBV	88479	283218	11.69%	1.334%
7	6.736	800	813	828	rBV2	536255	1642965	67.80%	7.737%
8	7.312	903	911	919	rVB2	14906	35039	1.45%	0.165%
9	7.441	924	933	940	rBV	18634	44932	1.85%	0.212%
10	8.177	1048	1058	1062	rBV	367580	875141	36.12%	4.121%
11	8.230	1062	1067	1080	rVB	553646	1267413	52.30%	5.969%
12	8.588	1114	1128	1139	rBV	331133	762740	31.48%	3.592%
13	9.112	1207	1217	1231	rBV2	1162907	2423193	100.00%	11.411%
14	9.347	1249	1257	1267	rVB2	62711	128924	5.32%	0.607%
15	10.576	1456	1466	1478	rBV	1154212	2217483	91.51%	10.443%
16	10.806	1498	1505	1522	rBV	1359190	2394567	98.82%	11.277%
17	10.953	1522	1530	1542	rVV	326534	568369	23.46%	2.677%
18	11.065	1545	1549	1564	rVV2	29238	59797	2.47%	0.282%
19	11.206	1567	1573	1581	rVV	120092	214885	8.87%	1.012%
20	11.871	1672	1686	1698	rBV	1126237	2092477	86.35%	9.854%
21	12.853	1846	1853	1863	rBV	845604	1491367	61.55%	7.023%
22	13.800	2006	2014	2023	rVB	841366	1454220	60.01%	6.848%

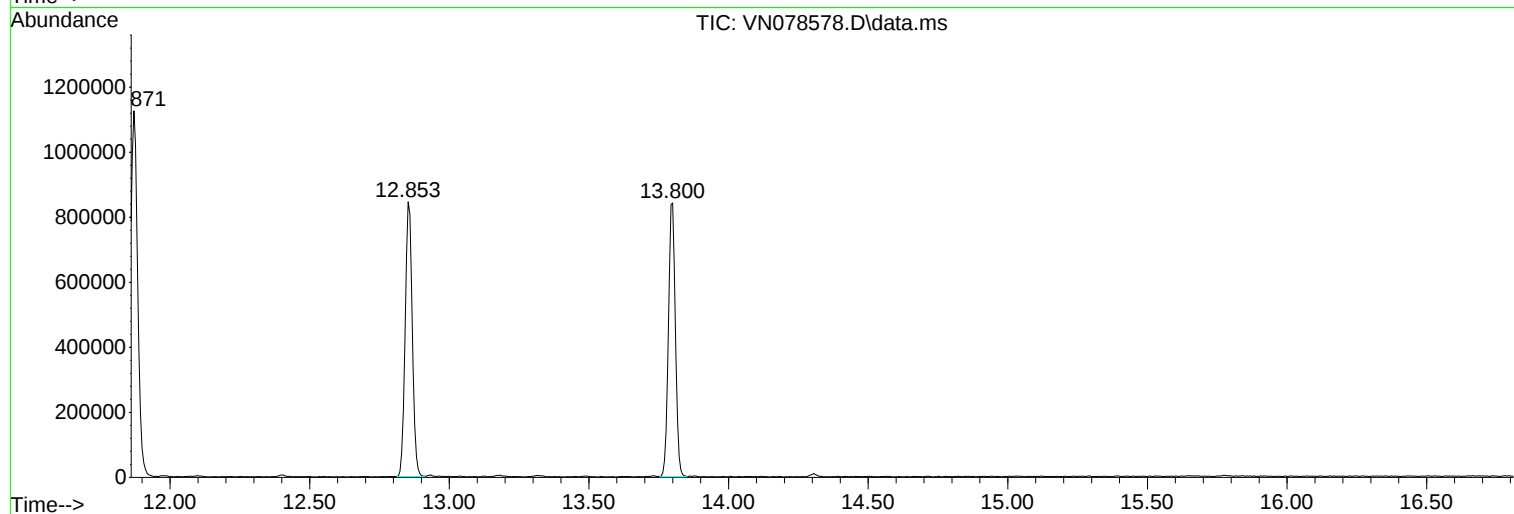
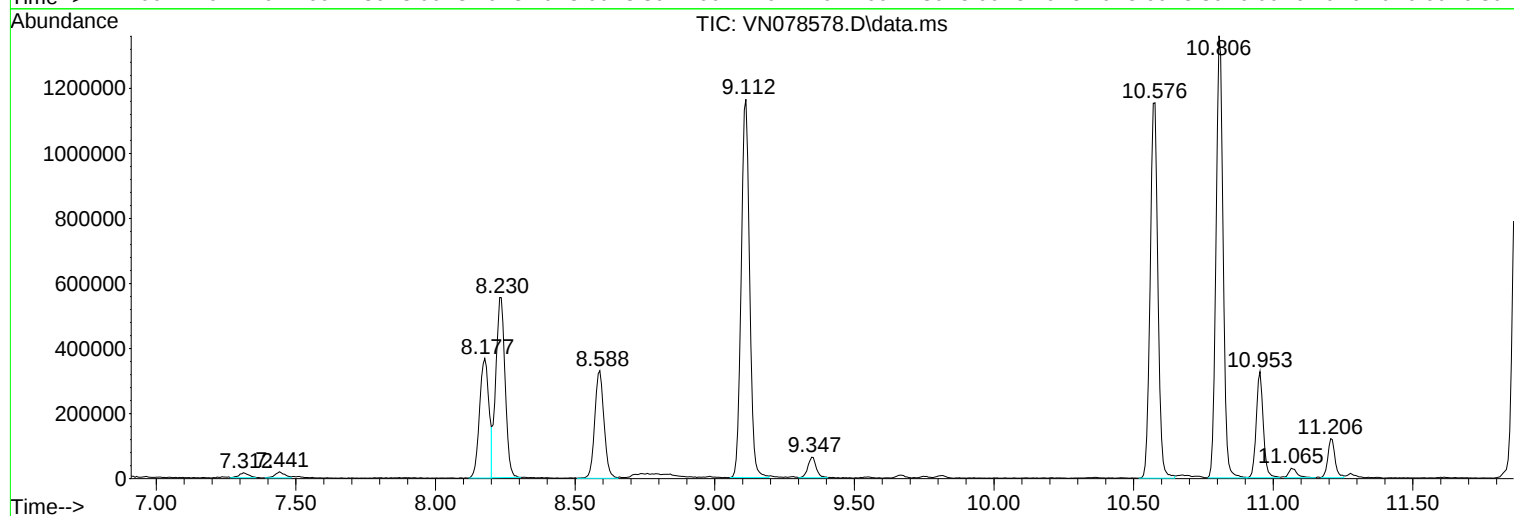
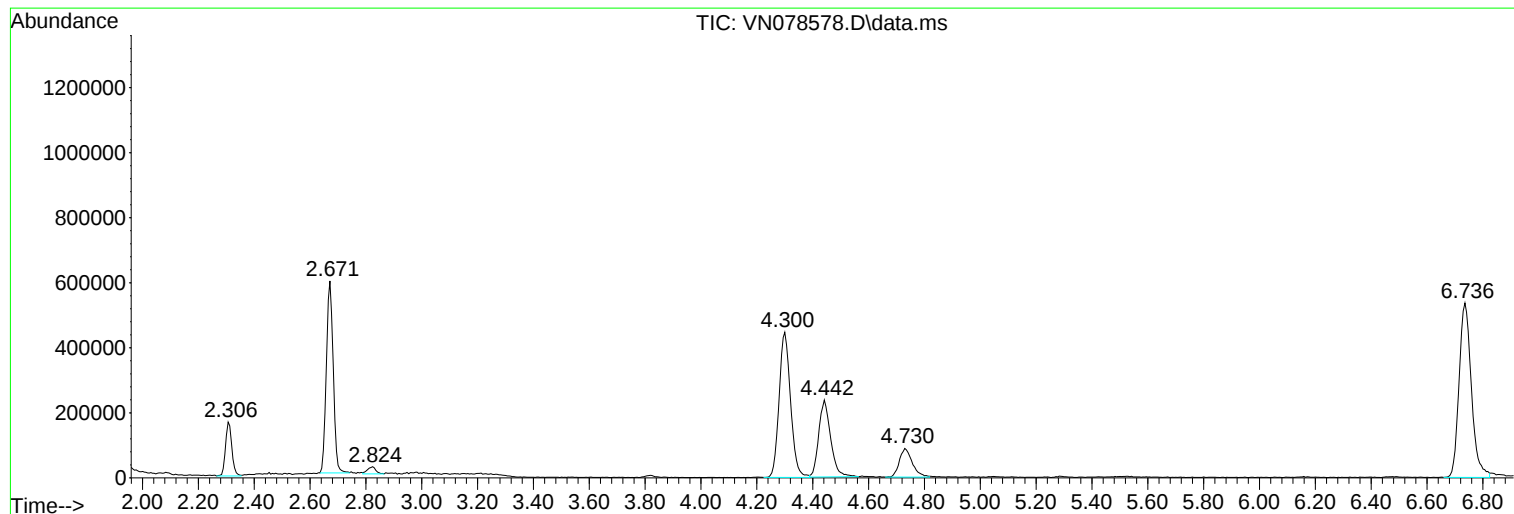
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.M
Quant Title : SW846 8260

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



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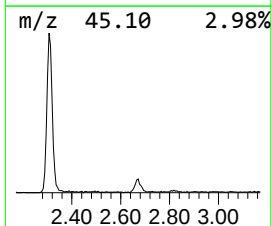
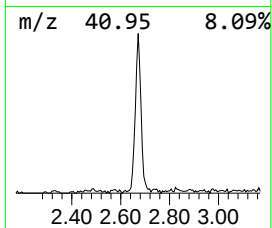
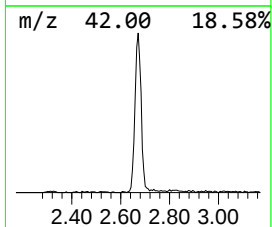
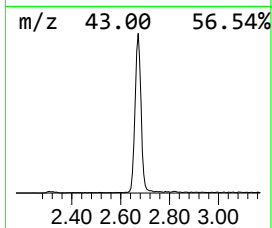
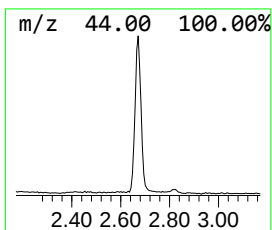
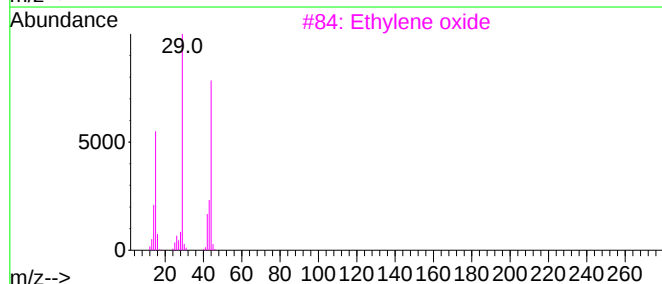
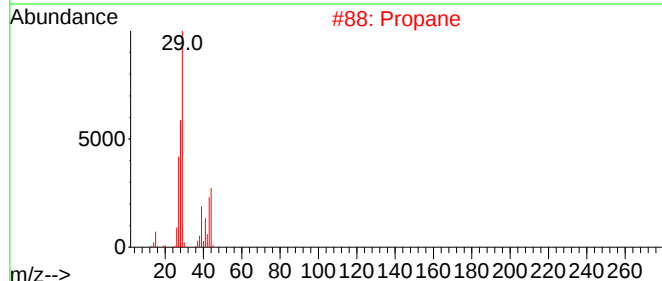
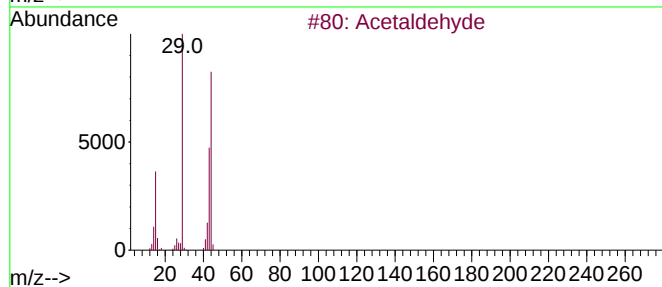
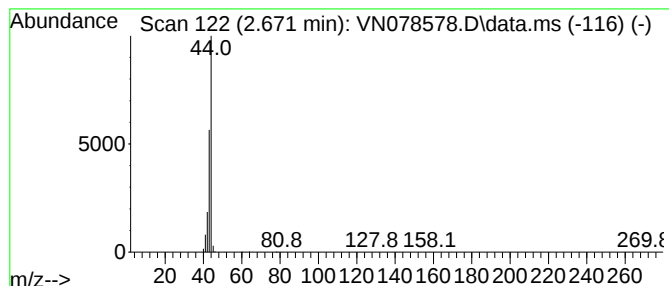
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.671	39.66 ug/l	1005200	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			1-Propanol, 2-amino-, (+/-)-	75	C3H9NO	006168-72-5	4
5			Alanine	89	C3H7NO2	000056-41-7	4



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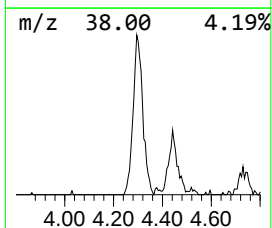
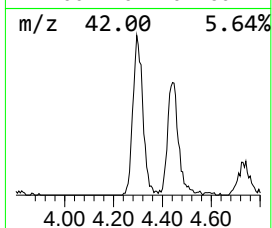
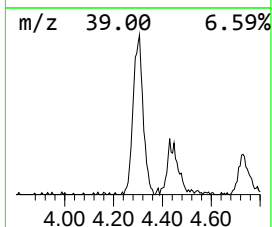
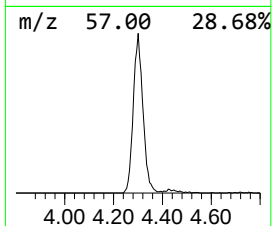
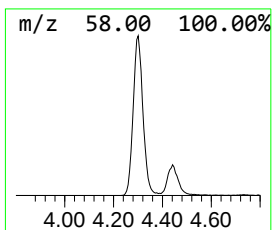
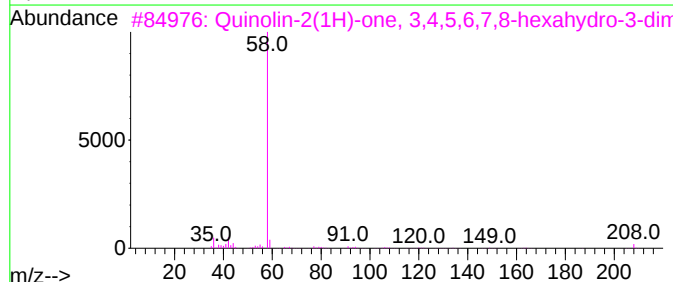
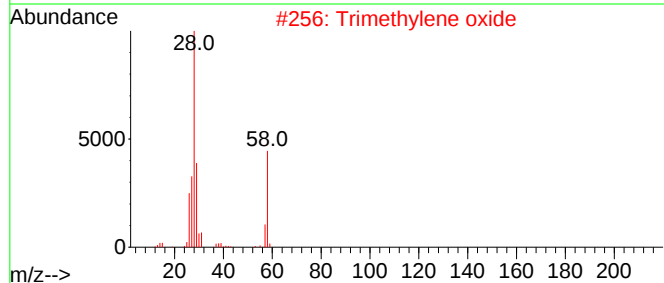
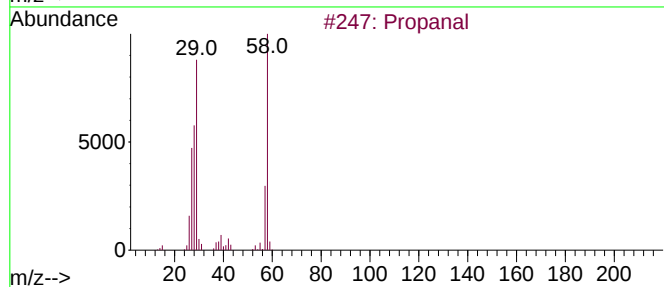
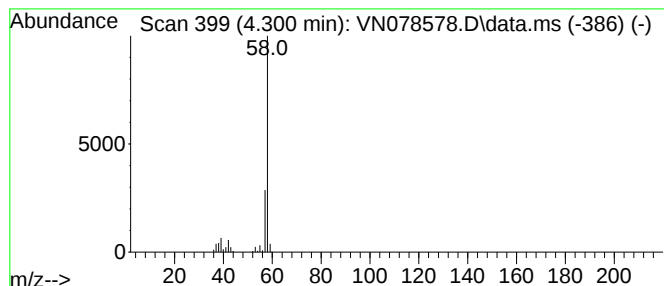
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.300	50.13 ug/l	1270690	Pentafluorobenzene	8.235

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	9
3			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
5			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7



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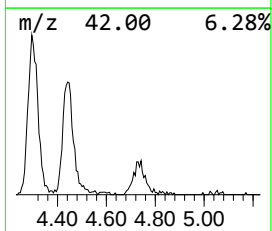
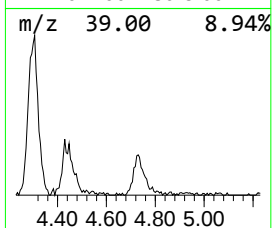
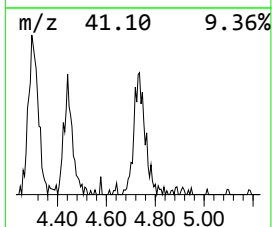
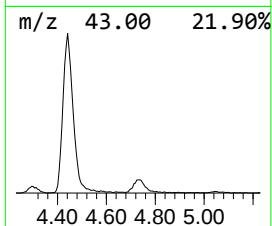
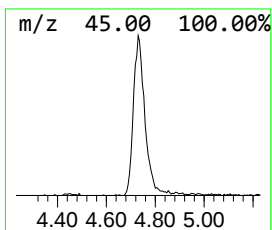
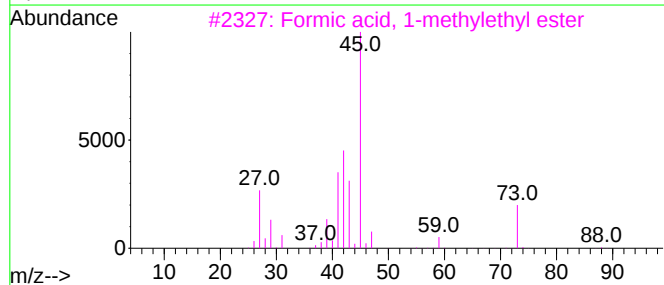
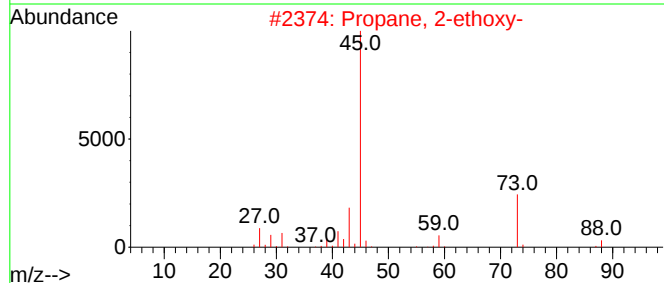
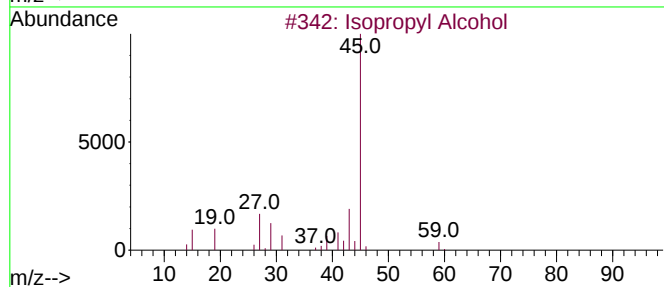
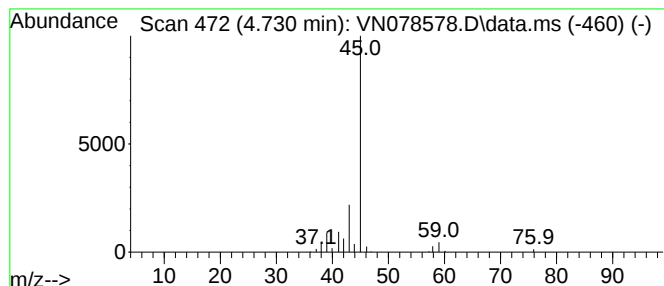
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Quant Title : SW846 8260

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

Peak Number 4 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.730	11.17 ug/l	283218	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	72
2			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	56
3			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
4			2-Pentanol	88	C5H12O	006032-29-7	9
5			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9



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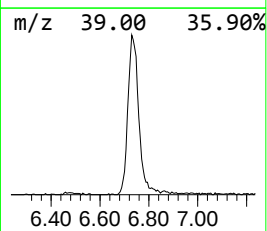
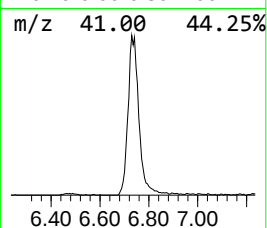
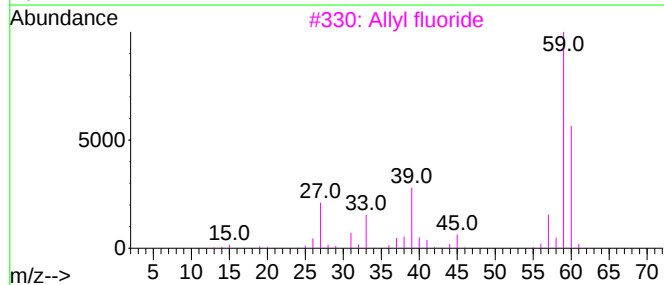
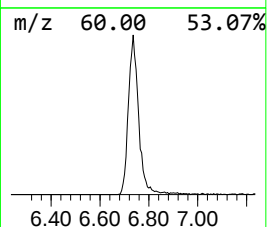
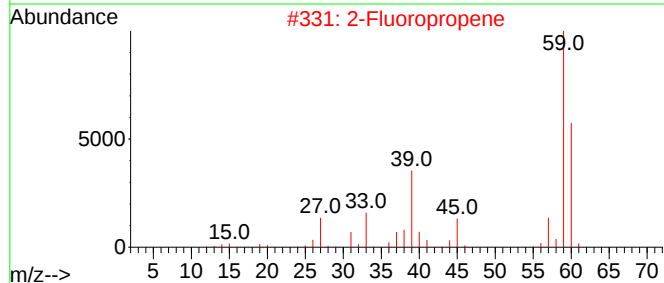
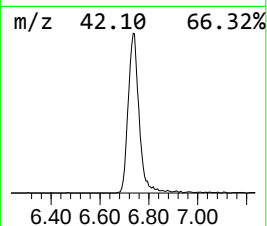
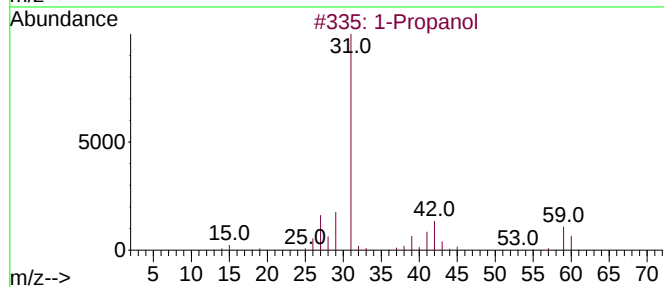
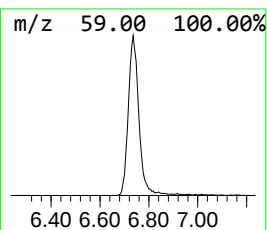
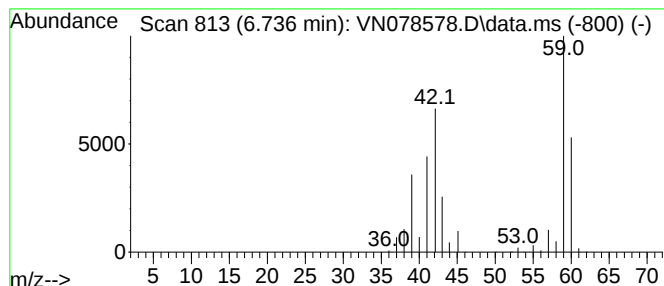
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.736	64.82 ug/l	1642970	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	72
2			2-Fluoropropene	60	C3H5F	001184-60-7	64
3			Allyl fluoride	60	C3H5F	000818-92-8	53
4			Formamidoxime	60	CH4N2O	000624-82-8	12
5			Cyclopropane	42	C3H6	000075-19-4	10



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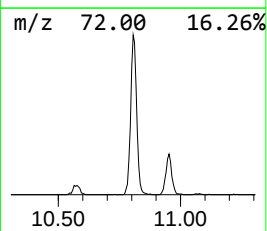
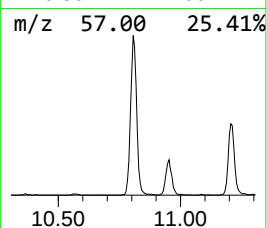
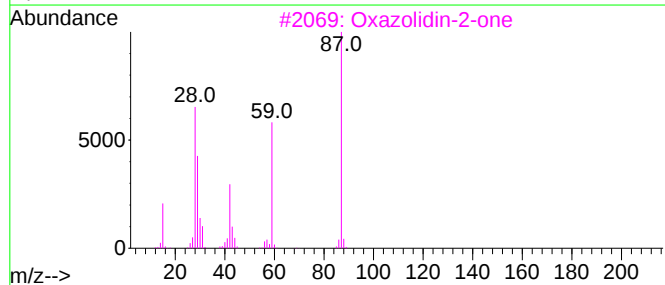
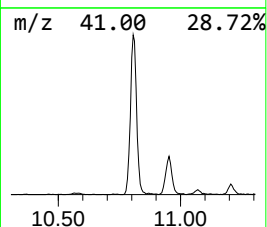
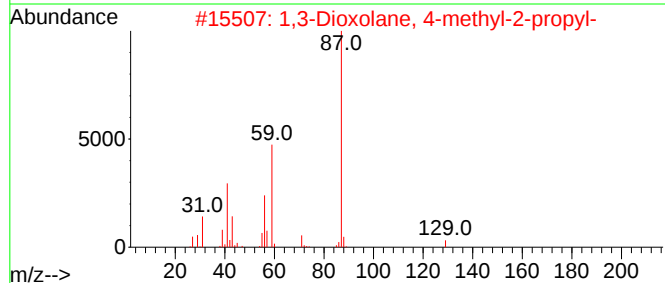
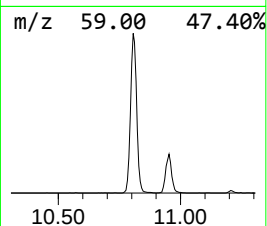
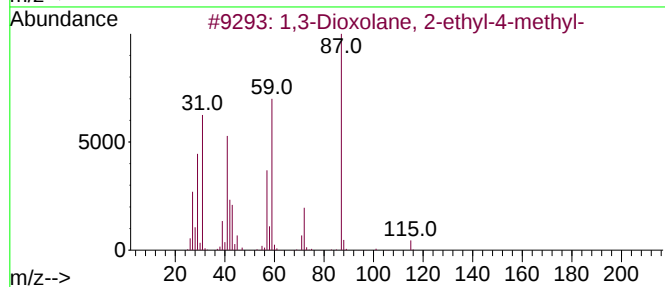
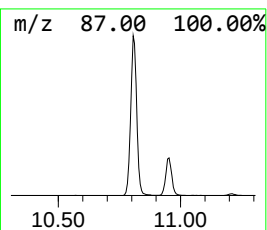
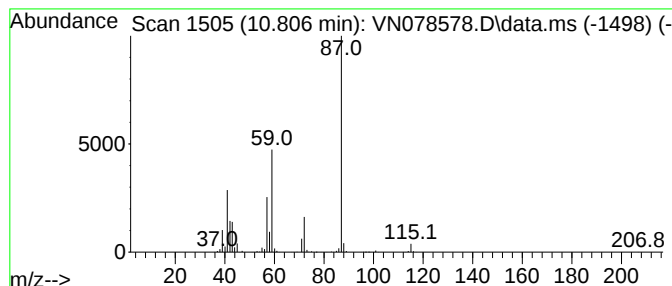
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Quant Title : SW846 8260

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Peak Number 6 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.806	57.22 ug/l	2394570	Chlorobenzene-d5		11.871	
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	59
3	Oxazolidin-2-one		87	C3H5NO2	000497-25-6	50
4	2-Propanone, O-methyloxime		87	C4H9NO	003376-35-0	50
5	Acetamide, N-ethyl-		87	C4H9NO	000625-50-3	50



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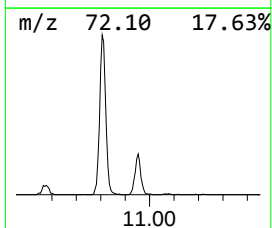
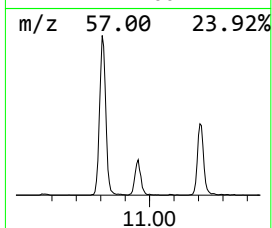
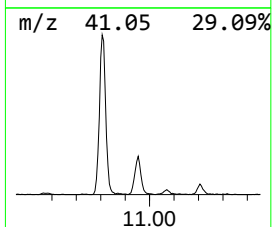
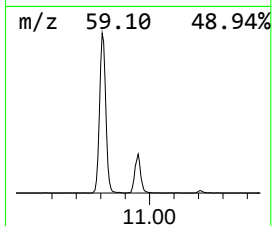
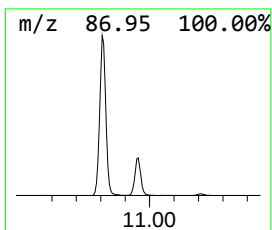
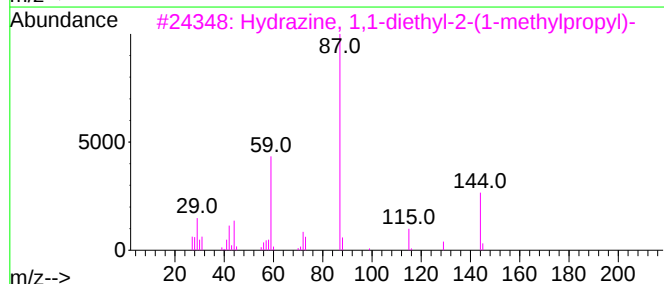
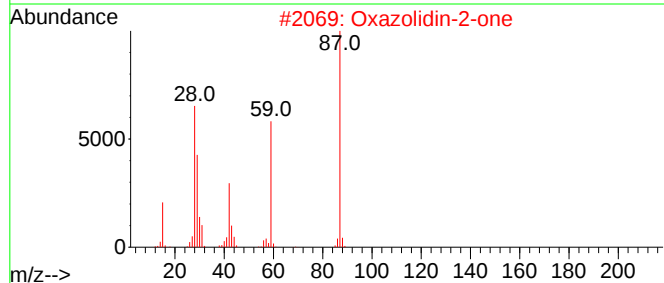
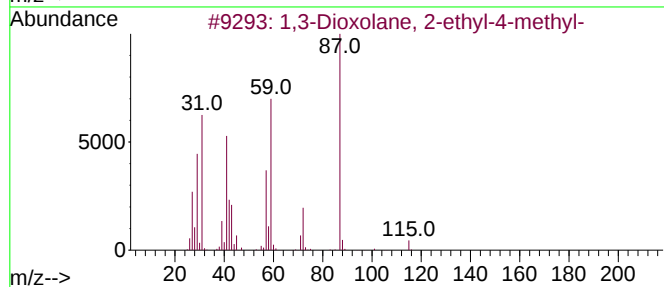
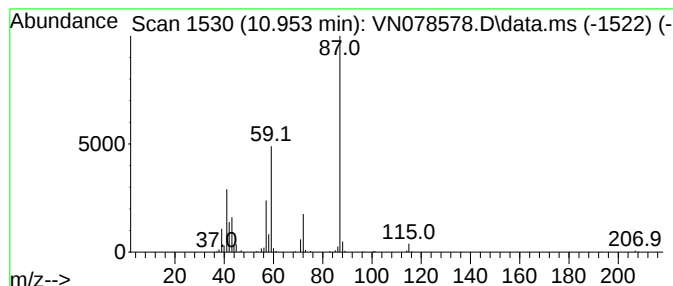
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Quant Title : SW846 8260

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

Peak Number 7 Oxazolidin-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.953	13.58 ug/l	568369	Chlorobenzene-d5	11.871

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	64
3			Hydrazine, 1,1-diethyl-2-(1-meth...	144	C8H20N2	067398-40-7	56
4			Hydrazine, 1,1-diethyl-2-(1-meth...	130	C7H18N2	067398-39-4	56
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071923\
Data File : VN078578.D
Acq On : 19 Jul 2023 14:12
Operator : JC\MD
Sample : 03664-05 200X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1012

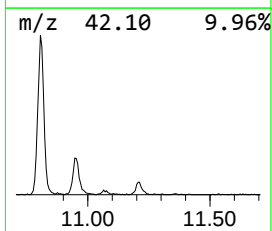
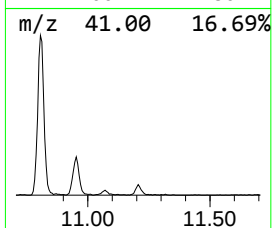
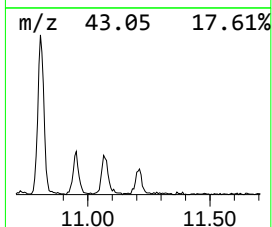
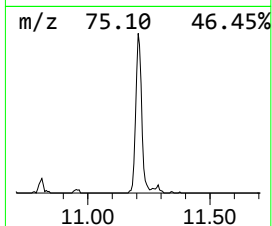
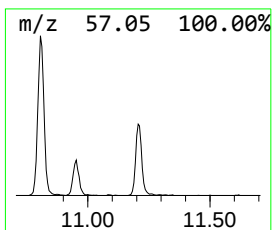
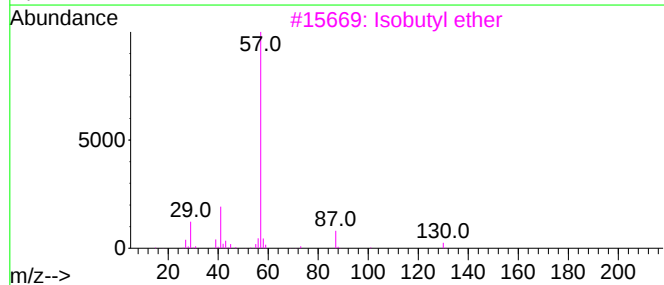
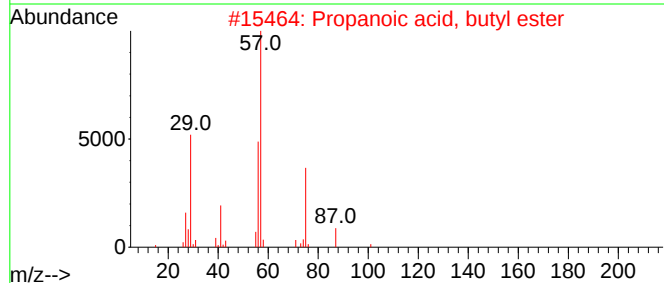
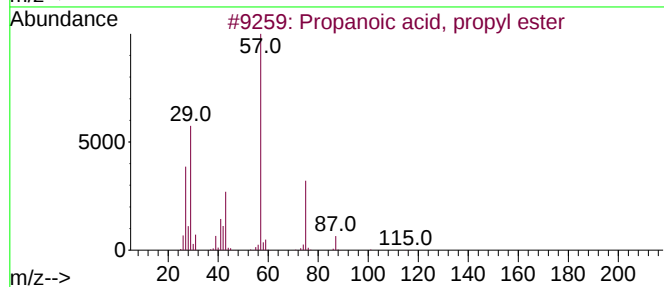
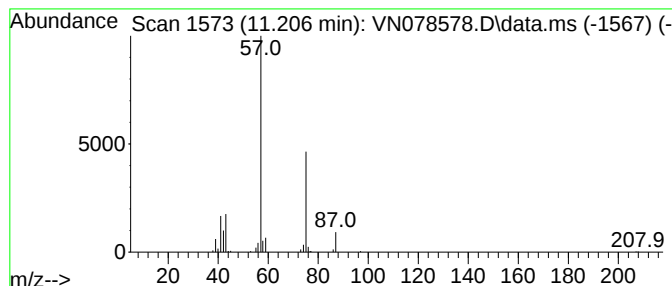
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.M
Quant Title : SW846 8260

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

Peak Number 8 Propanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	5.13 ug/l	214885	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39
3			Isobutyl ether	130	C8H18O	000628-55-7	10
4			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	10
5			Azetidine	57	C3H7N	000503-29-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071923\
Data File : VN078578.D
Acq On : 19 Jul 2023 14:12
Operator : JC\MD
Sample : 03664-05 200X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1012

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.671	39.7	ug/l	1005200	1	8.235	1267410	50.0
Propanal	4.300	50.1	ug/l	1270690	1	8.235	1267410	50.0
Isopropyl Alcohol	4.730	11.2	ug/l	283218	1	8.235	1267410	50.0
1-Propanol	6.736	64.8	ug/l	1642970	1	8.235	1267410	50.0
1,3-Dioxolane, ...	10.806	57.2	ug/l	2394570	3	11.871	2092480	50.0
Oxazolidin-2-one	10.953	13.6	ug/l	568369	3	11.871	2092480	50.0
Propanoic acid,...	11.206	5.1	ug/l	214885	3	11.871	2092480	50.0