

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111722\
 Data File : VN075304.D
 Acq On : 17 Nov 2022 15:18
 Operator : JC\MD
 Sample : N5675-07 10X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 AUD-1913

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\82N102622W.M
 Title : SW846 8260

Signal : TIC: VN075304.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.671	97	105	121	rBV	1393818	2565439	100.00%	18.874%
2	3.806	287	298	325	rBV	380619	1072583	41.81%	7.891%
3	4.295	370	381	395	rBV	164546	478190	18.64%	3.518%
4	4.436	395	405	421	rVB	34515	105413	4.11%	0.776%
5	6.730	784	795	809	rBV2	128959	415808	16.21%	3.059%
6	7.230	870	880	888	rBV4	33759	94506	3.68%	0.695%
7	8.171	1030	1040	1044	rBV	126235	285907	11.14%	2.103%
8	8.230	1044	1050	1059	rVB	220410	497889	19.41%	3.663%
9	8.530	1092	1101	1106	rBV	178856	421104	16.41%	3.098%
10	8.583	1106	1110	1123	rVB	136037	290079	11.31%	2.134%
11	9.106	1190	1199	1219	rBV	1211709	2470516	96.30%	18.176%
12	9.265	1219	1226	1233	rBV	108942	223488	8.71%	1.644%
13	9.341	1233	1239	1248	rVB	135662	269272	10.50%	1.981%
14	10.565	1439	1447	1458	rBV	501726	966233	37.66%	7.109%
15	10.800	1479	1487	1502	rBV	494232	855572	33.35%	6.294%
16	10.947	1505	1512	1523	rBV3	118793	223690	8.72%	1.646%
17	11.212	1550	1557	1565	rBV	22419	58900	2.30%	0.433%
18	11.818	1651	1660	1662	rBV3	21808	35681	1.39%	0.263%
19	11.865	1662	1668	1678	rVB	450923	790998	30.83%	5.819%
20	12.100	1700	1708	1715	rBV	27162	47466	1.85%	0.349%
21	12.847	1828	1835	1845	rVB	343412	569521	22.20%	4.190%
22	13.788	1988	1995	2003	rBV	419861	744036	29.00%	5.474%
23	13.876	2003	2010	2016	rBV	63507	110204	4.30%	0.811%

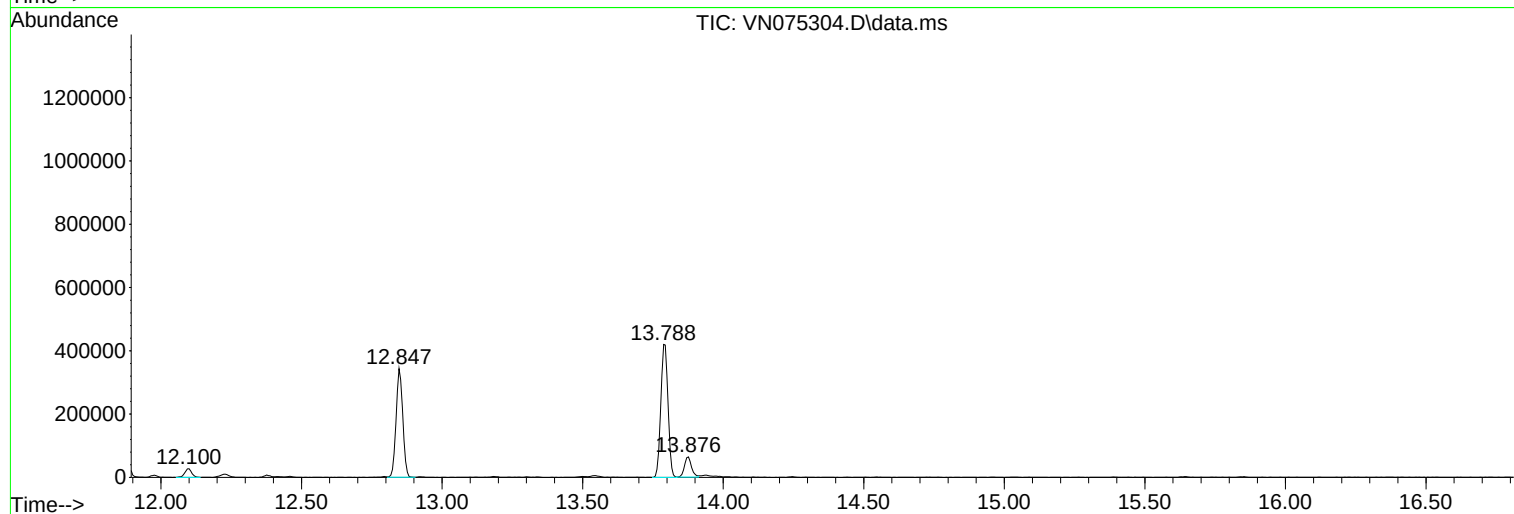
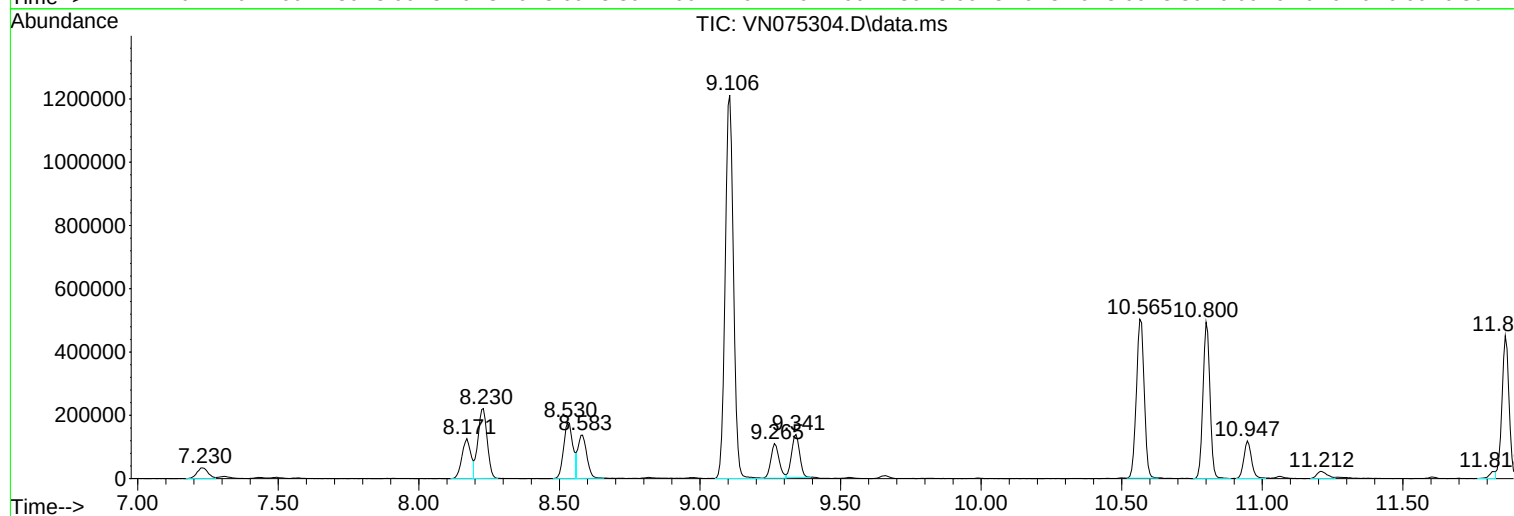
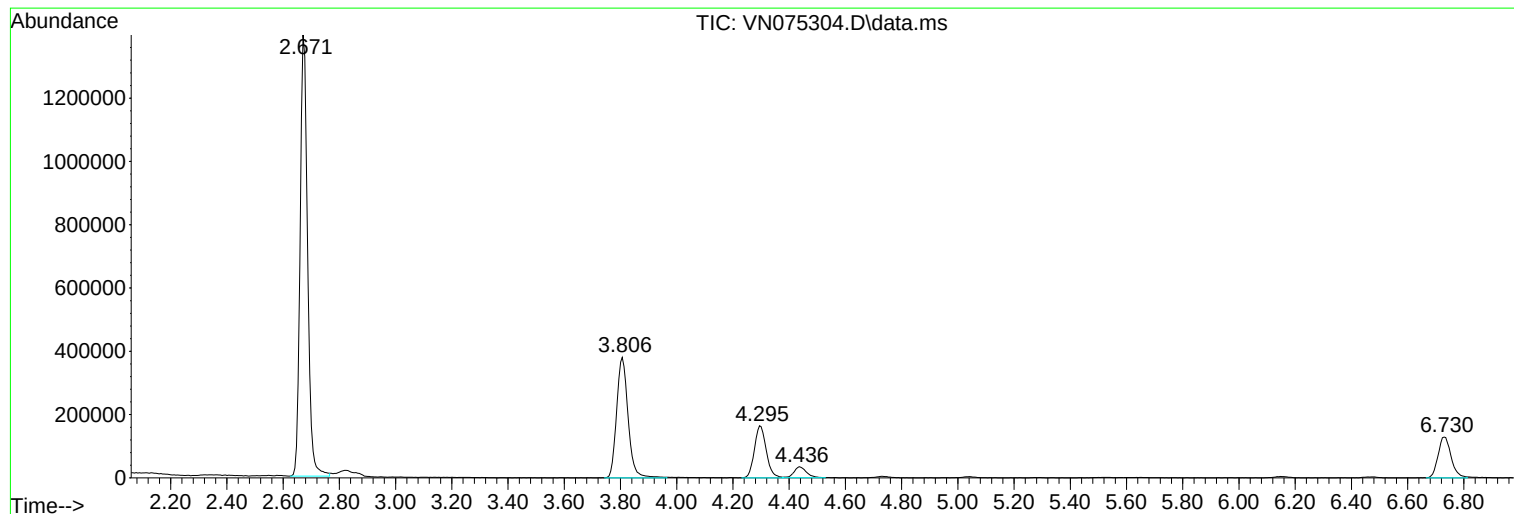
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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



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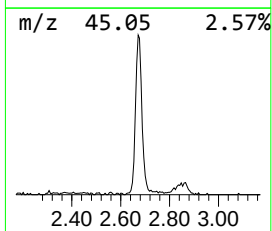
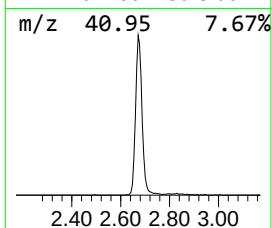
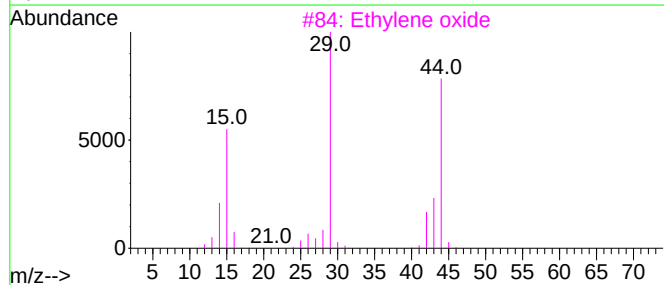
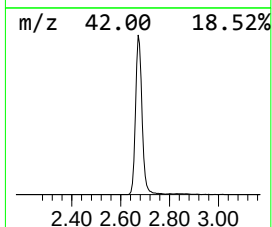
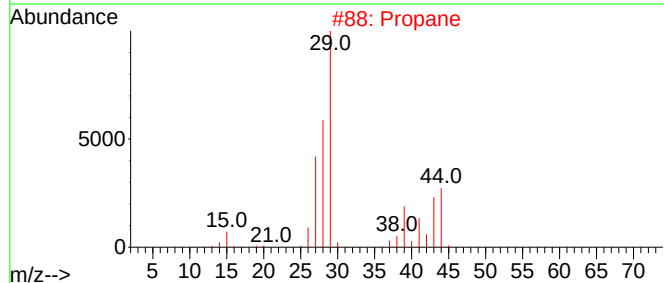
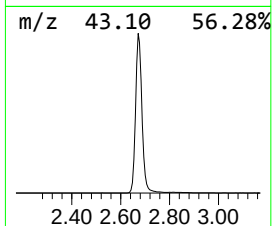
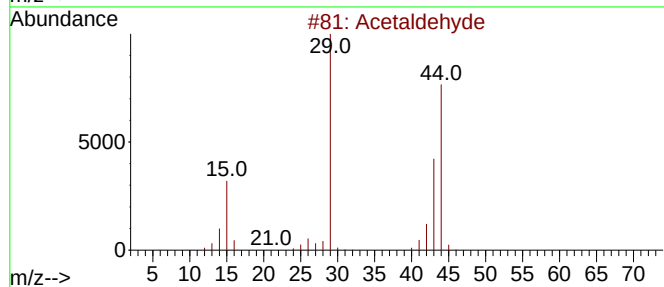
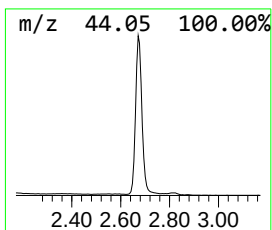
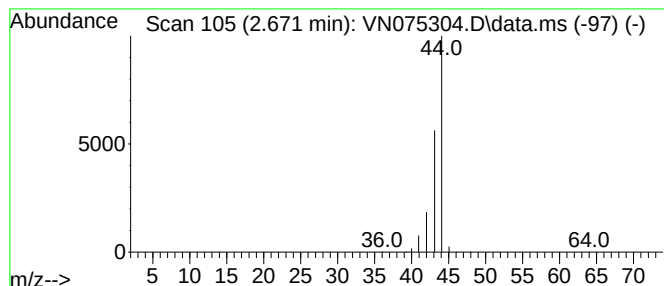
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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.
2.671	257.63 ug/l	2565440	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
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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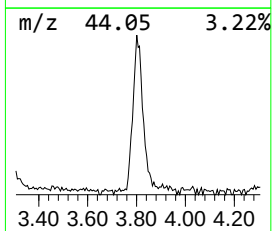
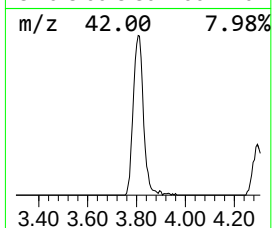
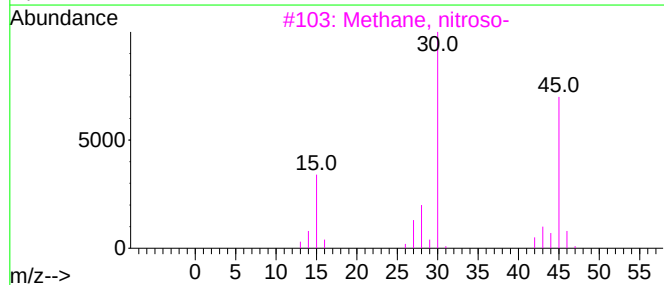
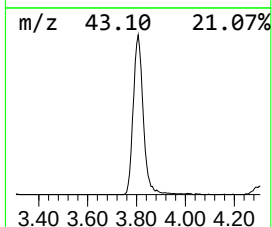
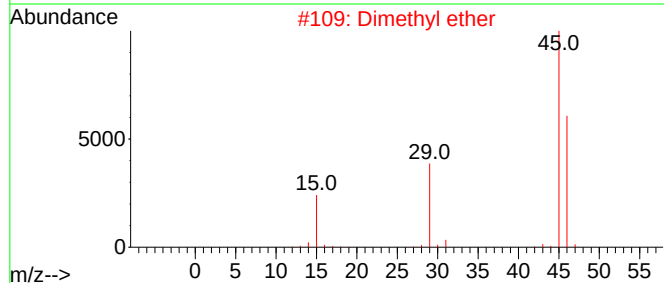
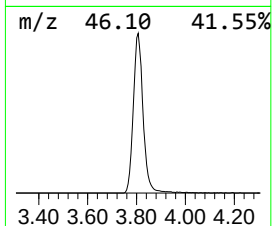
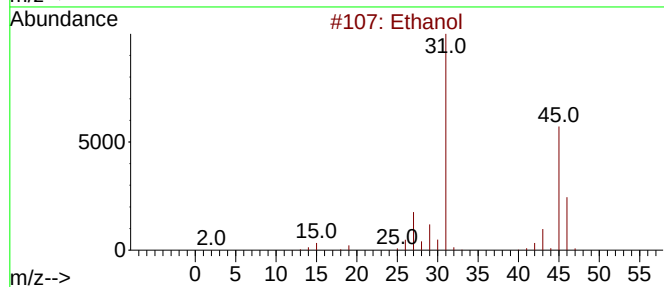
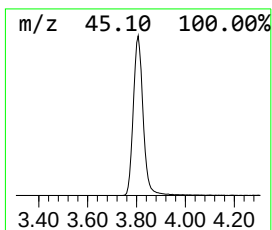
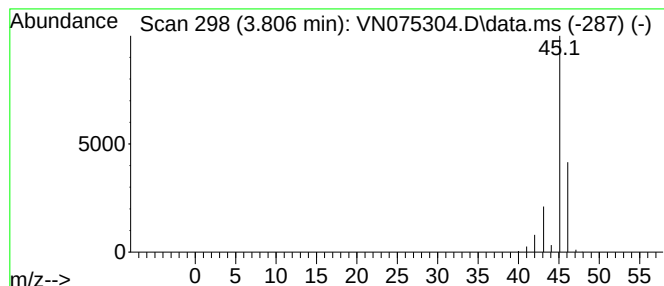
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.806	107.71 ug/l	1072580	Pentafluorobenzene	8.230

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	Oxalic acid			90	C2H2O4	000144-62-7	4



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1913

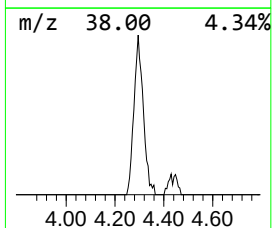
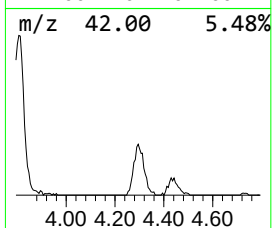
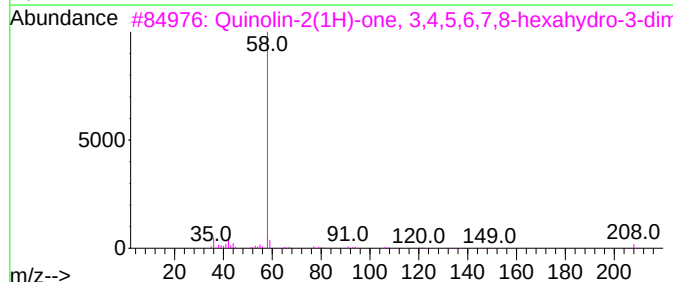
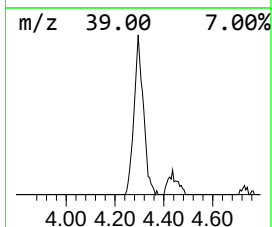
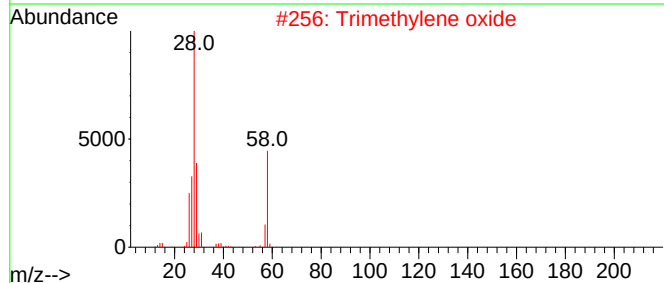
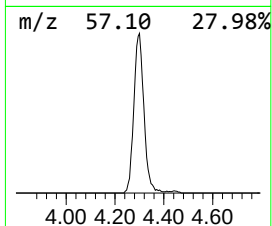
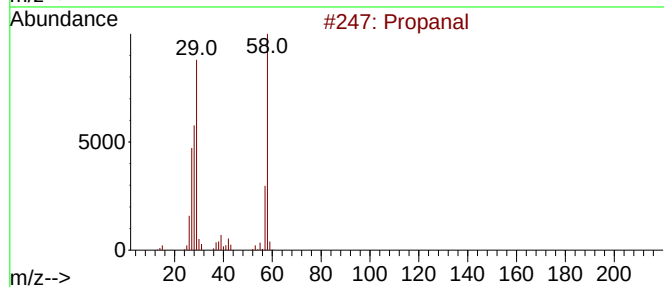
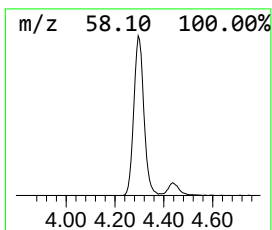
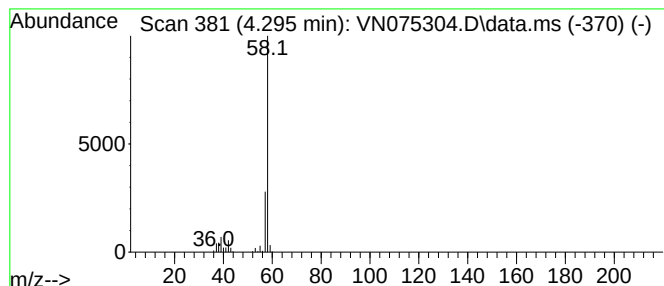
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.295	48.02 ug/l	478190	Pentafluorobenzene	8.230

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	7



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ALS Vial : 8 Sample Multiplier: 1

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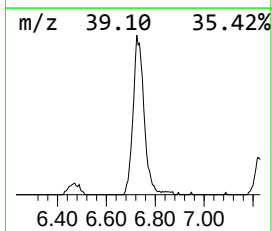
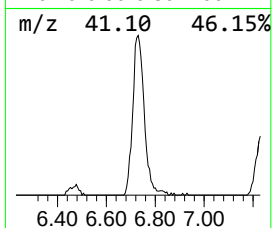
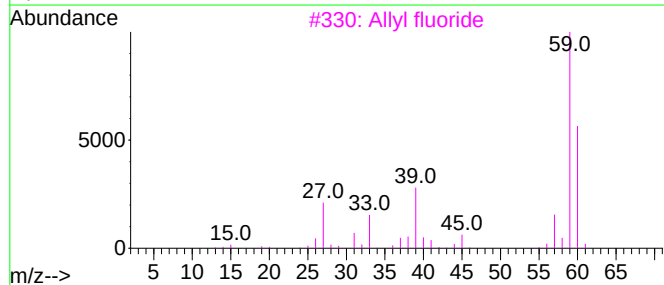
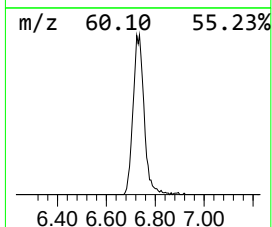
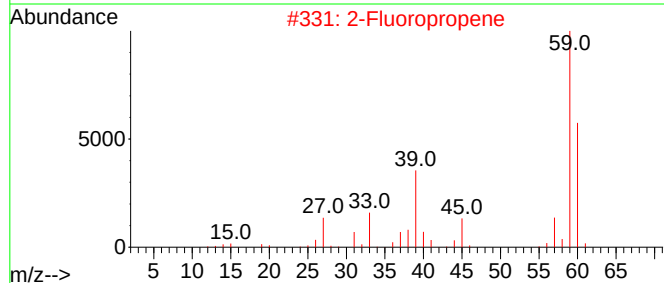
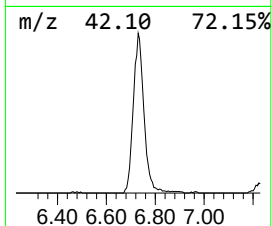
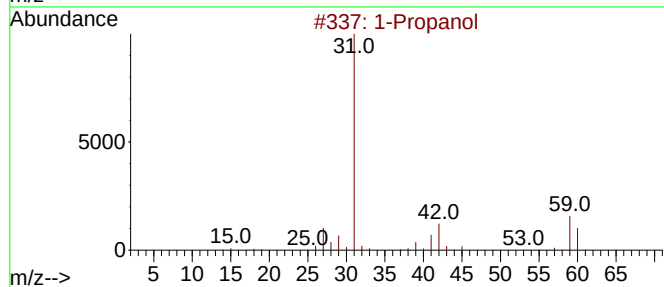
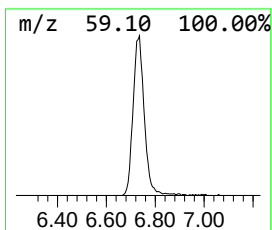
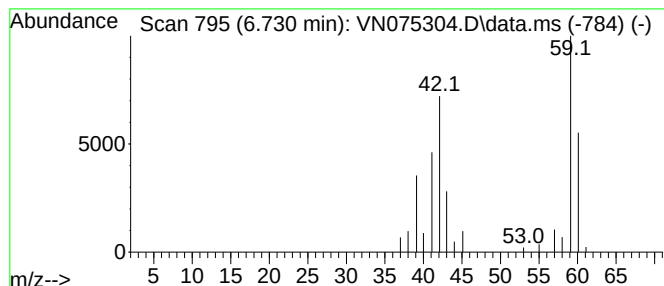
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Quant Title : SW846 8260

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

Peak Number 4 1-Propanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.730	41.76 ug/l	415808	Pentafluorobenzene	8.230

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	Cyclopropane		42	C3H6	000075-19-4	10
5	Formamidoxime		60	CH4N2O	000624-82-8	9



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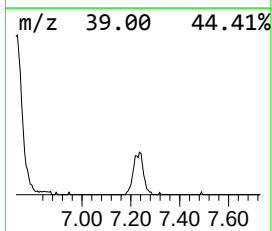
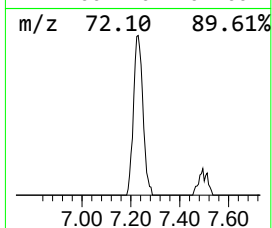
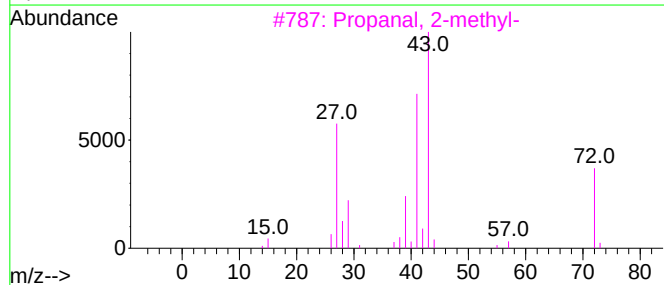
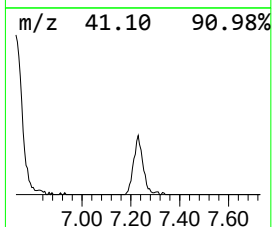
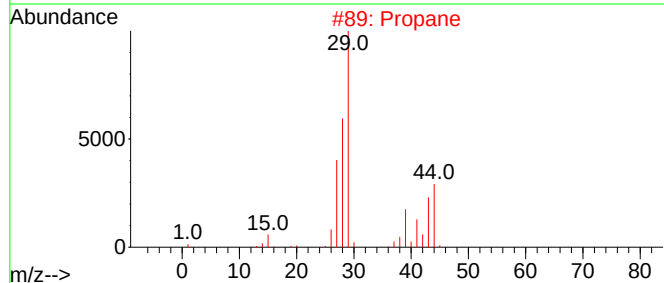
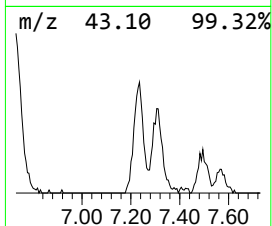
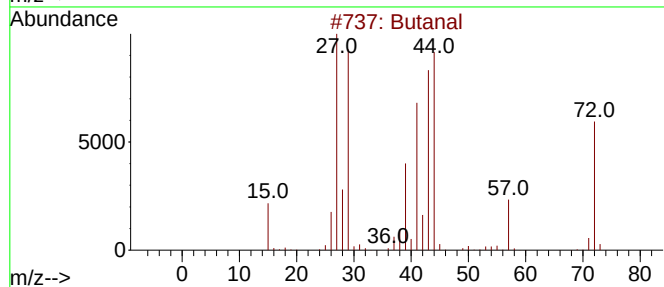
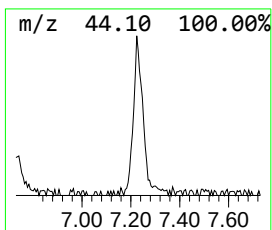
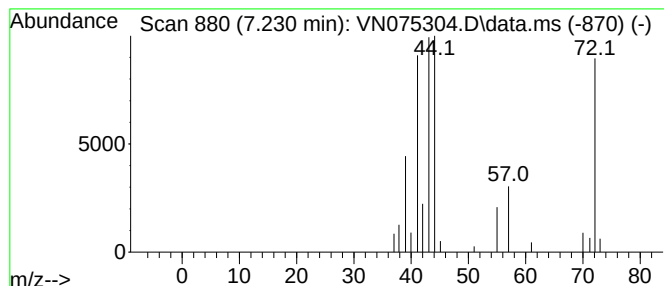
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Quant Title : SW846 8260

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

Peak Number 5 Butanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.230	9.49 ug/l	94506	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propane	44	C3H8	000074-98-6	47
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	32



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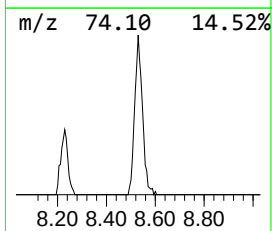
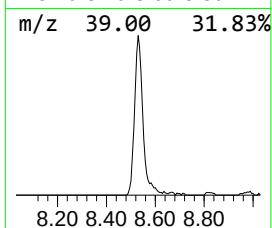
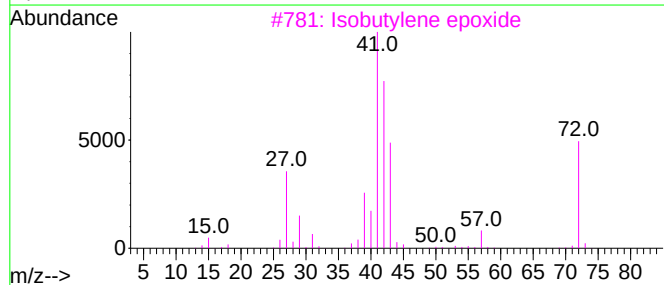
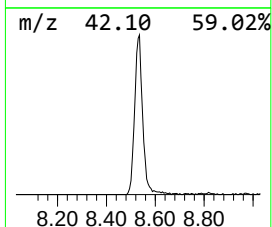
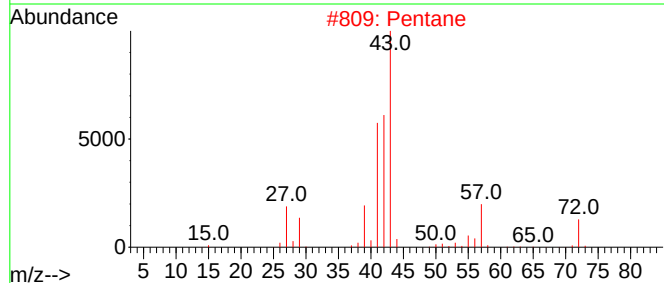
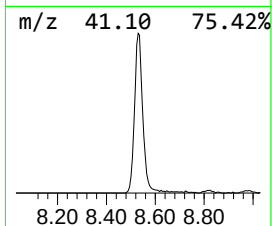
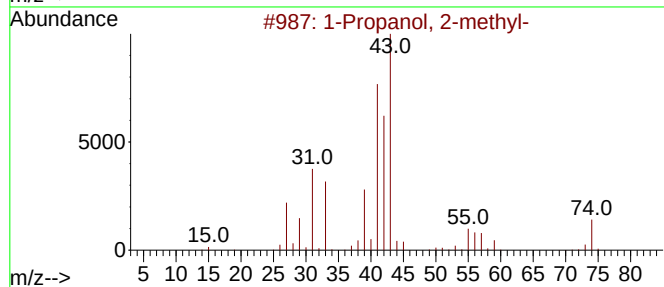
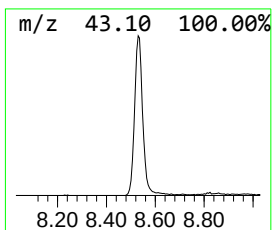
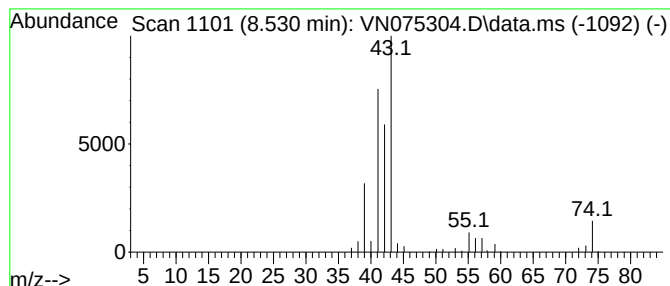
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Quant Title : SW846 8260

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

Peak Number 6 1-Propanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.530	42.29 ug/l	421104	Pentafluorobenzene	8.230

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	91	
2	Pentane	72	C5H12	000109-66-0	45	
3	Isobutylene epoxide	72	C4H8O	000558-30-5	40	
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	35	
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	17	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111722\
Data File : VN075304.D
Acq On : 17 Nov 2022 15:18
Operator : JC\MD
Sample : N5675-07 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1913

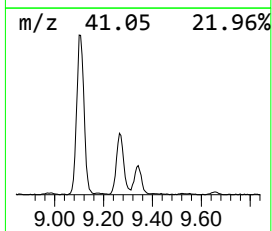
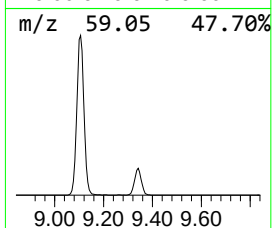
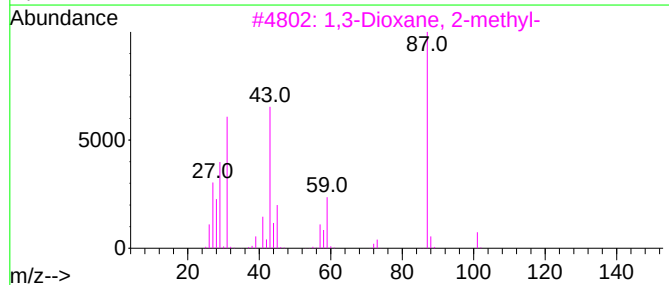
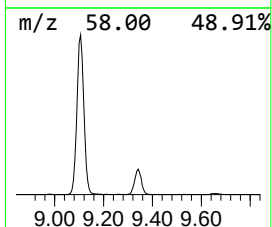
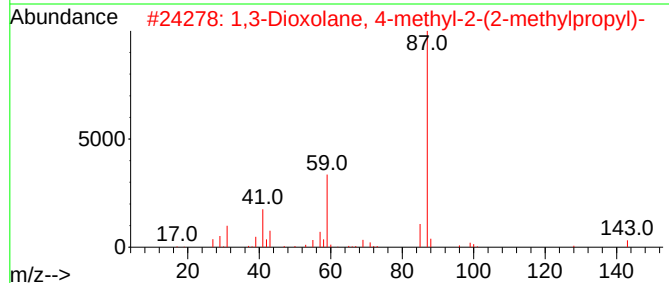
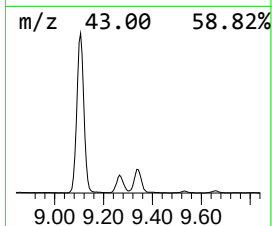
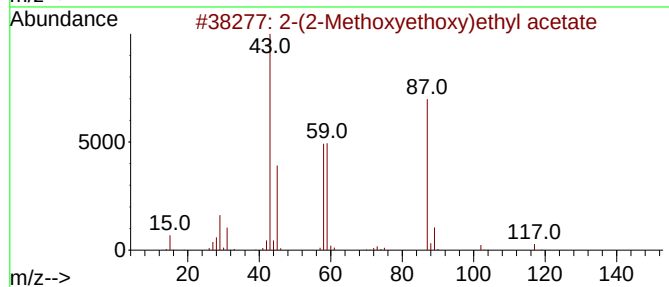
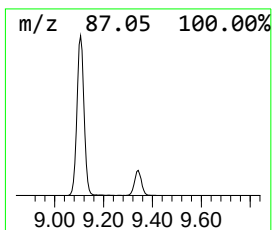
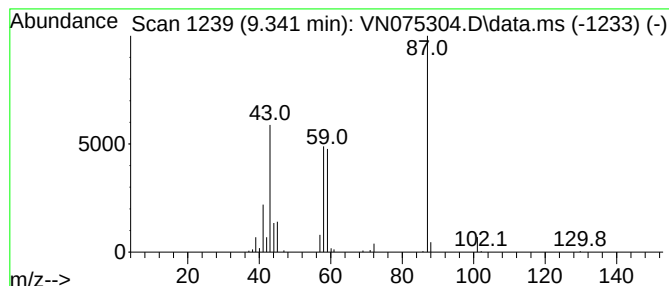
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Quant Title : SW846 8260

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

Peak Number 7 2-(2-Methoxyethoxy)ethyl ac... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.341	5.45 ug/l	269272	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	56
2			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	50
3			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	49
4			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
5			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111722\
Data File : VN075304.D
Acq On : 17 Nov 2022 15:18
Operator : JC\MD
Sample : N5675-07 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

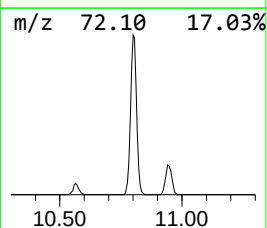
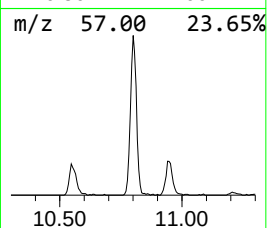
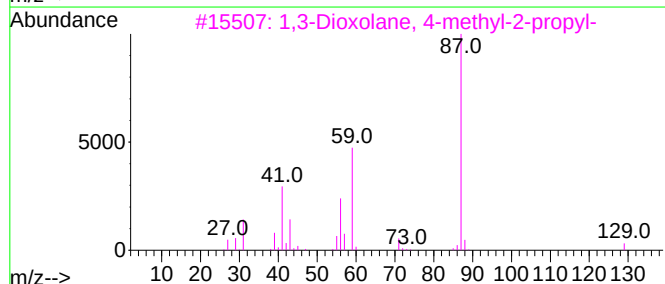
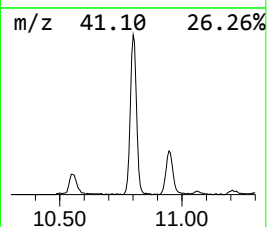
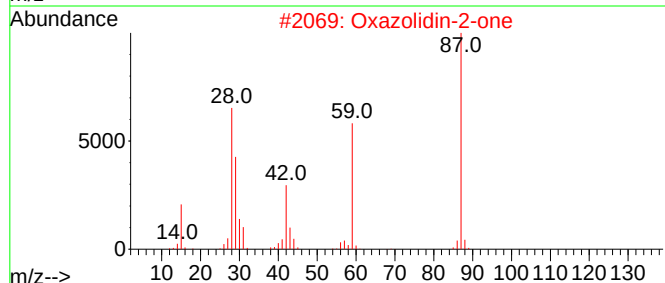
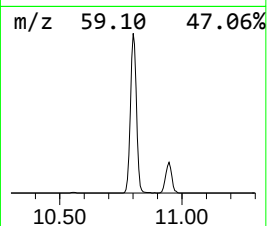
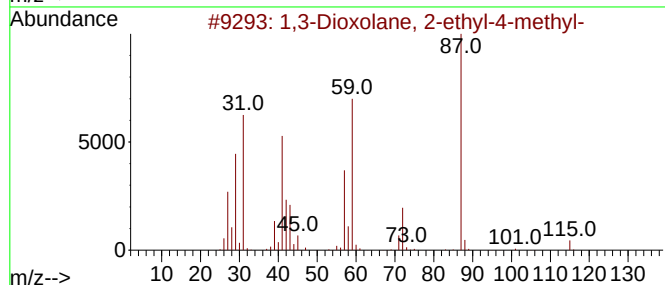
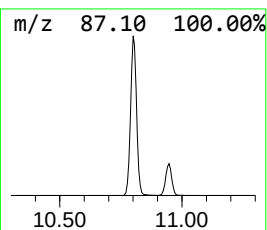
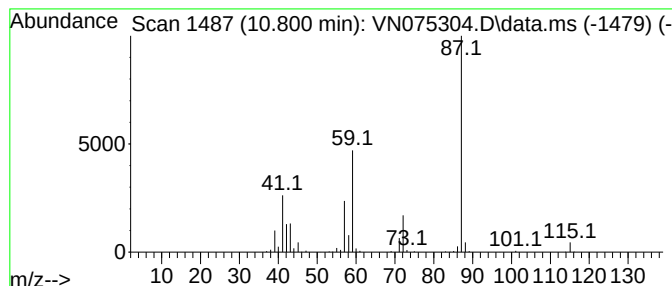
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MSVOA_N
ClientSampleId :
AUD-1913

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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

Peak Number 8 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.800	54.08 ug/l	855572	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	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64
4	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	56
5	2-Propanone, 0-methyloxime	87	C4H9NO	003376-35-0	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111722\
Data File : VN075304.D
Acq On : 17 Nov 2022 15:18
Operator : JC\MD
Sample : N5675-07 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1913

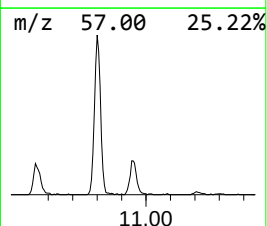
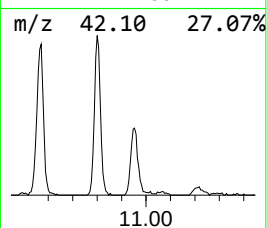
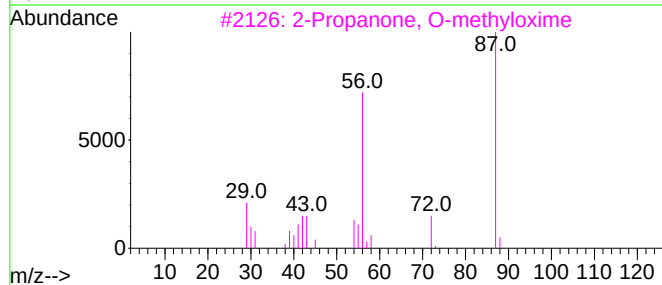
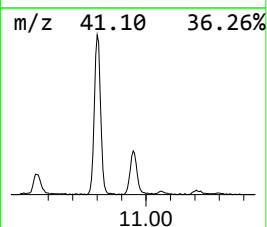
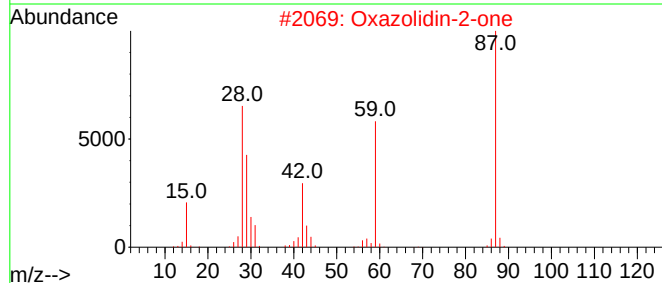
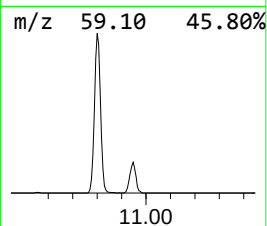
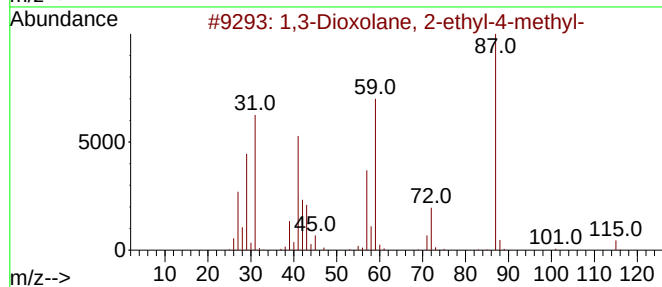
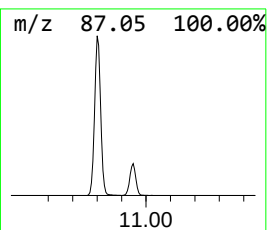
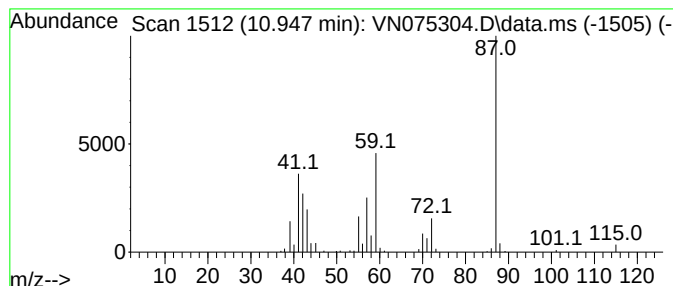
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Quant Title : SW846 8260

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

Peak Number 9 Oxazolidin-2-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	14.14 ug/l	223690	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	72
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
3			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	47
4			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	45
5			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111722\
Data File : VN075304.D
Acq On : 17 Nov 2022 15:18
Operator : JC\MD
Sample : N5675-07 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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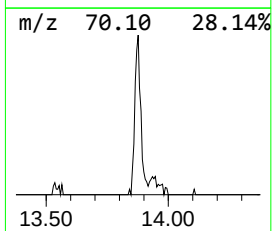
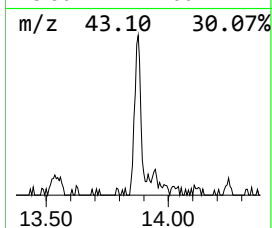
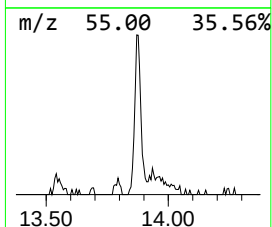
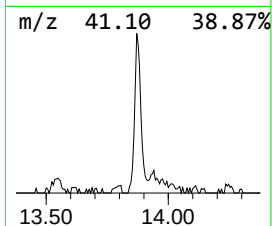
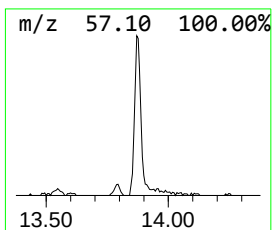
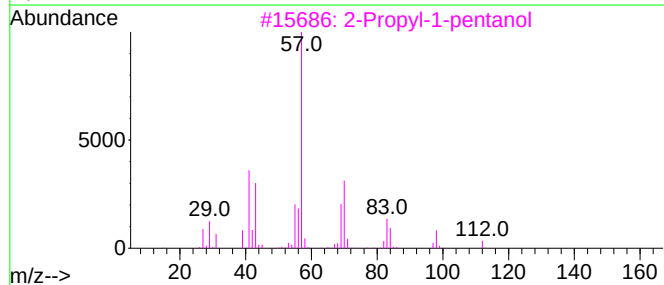
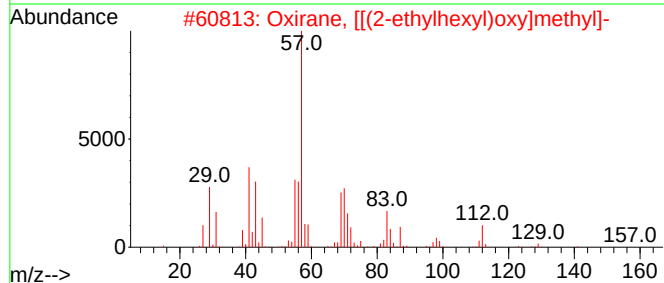
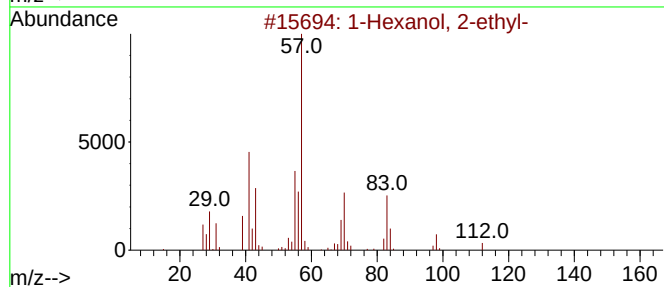
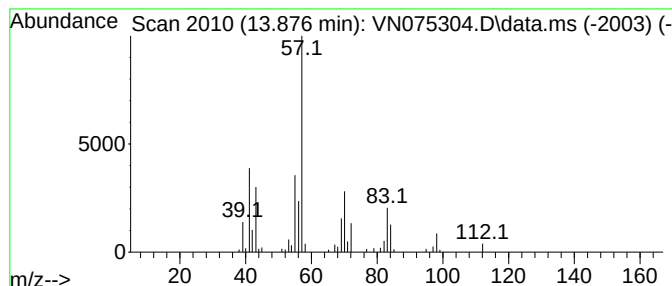
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Quant Title : SW846 8260

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	7.41 ug/l	110204	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	64
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
4			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111722\
Data File : VN075304.D
Acq On : 17 Nov 2022 15:18
Operator : JC\MD
Sample : N5675-07 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1913

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.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	2.671	257.6	ug/l	2565440	1	8.230	497889	50.0
Ethanol	3.806	107.7	ug/l	1072580	1	8.230	497889	50.0
Propanal	4.295	48.0	ug/l	478190	1	8.230	497889	50.0
1-Propanol	6.730	41.8	ug/l	415808	1	8.230	497889	50.0
Butanal	7.230	9.5	ug/l	94506	1	8.230	497889	50.0
1-Propanol, 2-m...	8.530	42.3	ug/l	421104	1	8.230	497889	50.0
2-(2-Methoxyeth...	9.341	5.5	ug/l	269272	2	9.106	2470520	50.0
1,3-Dioxolane, ...	10.800	54.1	ug/l	855572	3	11.865	790998	50.0
Oxazolidin-2-one	10.947	14.1	ug/l	223690	3	11.865	790998	50.0
1-Hexanol, 2-et...	13.876	7.4	ug/l	110204	4	13.788	744036	50.0