

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
 Data File : VX030377.D
 Acq On : 03 Aug 2022 17:44
 Operator : JC/MD
 Sample : N4018-03 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 33773-74

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_X\Method\82X072522W.M
 Title : SW846 8260

Signal : TIC: VX030377.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	17	rVB2	14164	14346	1.66%	0.223%
2	1.453	56	60	72	rBV	53779	66865	7.72%	1.040%
3	1.575	72	80	81	rBV4	4870	10518	1.21%	0.164%
4	2.075	155	162	170	rBV	158346	262413	30.30%	4.082%
5	2.294	192	198	208	rVV	98636	153267	17.70%	2.384%
6	2.386	208	213	223	rVB	26564	42993	4.96%	0.669%
7	2.788	274	279	286	rVB2	6619	11888	1.37%	0.185%
8	2.946	297	305	315	rBV2	16704	39468	4.56%	0.614%
9	3.873	448	457	472	rBV	215167	562349	64.94%	8.748%
10	4.593	564	575	589	rBV2	9048	30475	3.52%	0.474%
11	5.391	695	706	717	rBV	101204	296667	34.26%	4.615%
12	5.556	721	733	746	rVV	113444	328993	37.99%	5.118%
13	5.964	790	800	813	rBV	125473	329348	38.03%	5.124%
14	6.769	922	932	943	rBV	193635	472562	54.57%	7.352%
15	6.885	943	951	961	rVB	64319	163501	18.88%	2.544%
16	7.214	998	1005	1013	rBV2	36945	78203	9.03%	1.217%
17	7.293	1013	1018	1025	rVB5	8055	17618	2.03%	0.274%
18	8.653	1233	1241	1249	rBV	563888	865985	100.00%	13.472%
19	8.720	1249	1252	1258	rVB4	5016	8927	1.03%	0.139%
20	9.000	1289	1298	1310	rBV	291066	429593	49.61%	6.683%
21	9.165	1318	1325	1332	rBV	188826	262917	30.36%	4.090%
22	10.055	1465	1471	1483	rBV	404621	569808	65.80%	8.865%
23	10.165	1483	1489	1501	rBV4	6784	15309	1.77%	0.238%
24	10.305	1507	1512	1518	rVB5	7452	12035	1.39%	0.187%
25	10.402	1523	1528	1532	rBV2	6872	9776	1.13%	0.152%
26	10.738	1578	1583	1591	rVB5	7195	11289	1.30%	0.176%
27	11.085	1634	1640	1647	rBV	434268	561188	64.80%	8.730%
28	11.152	1647	1651	1656	rVB2	8687	11922	1.38%	0.185%
29	11.664	1724	1735	1743	rBV6	10090	18667	2.16%	0.290%
30	11.902	1765	1774	1780	rBV4	10368	23714	2.74%	0.369%
31	12.024	1789	1794	1802	rVB	581825	698863	80.70%	10.872%
32	12.225	1822	1827	1832	rBV2	7986	15139	1.75%	0.236%
33	12.286	1832	1837	1838	rBV4	8791	12012	1.39%	0.187%
34	13.780	2077	2082	2088	rVB	12848	19334	2.23%	0.301%

Sum of corrected areas: 6427952

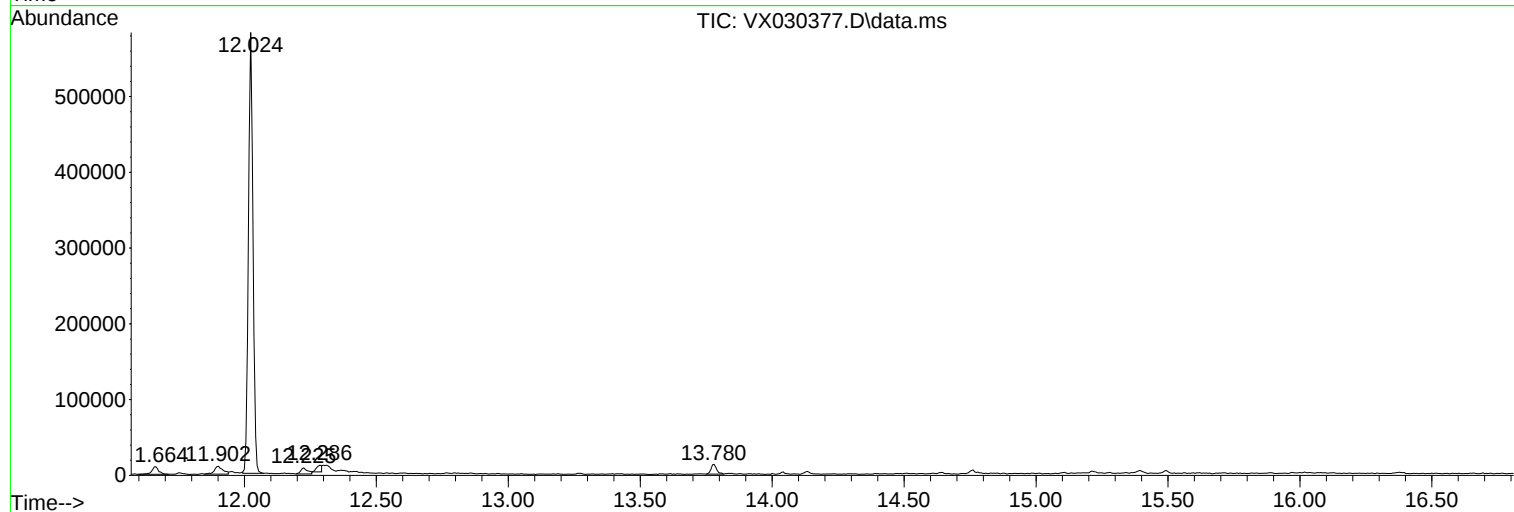
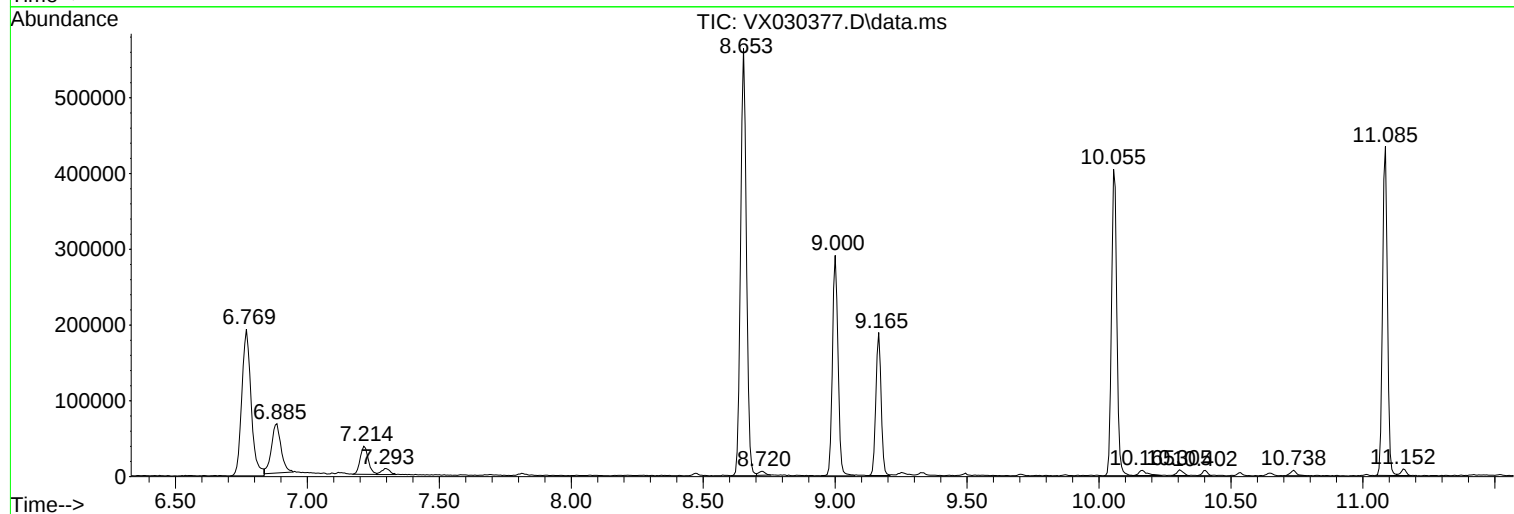
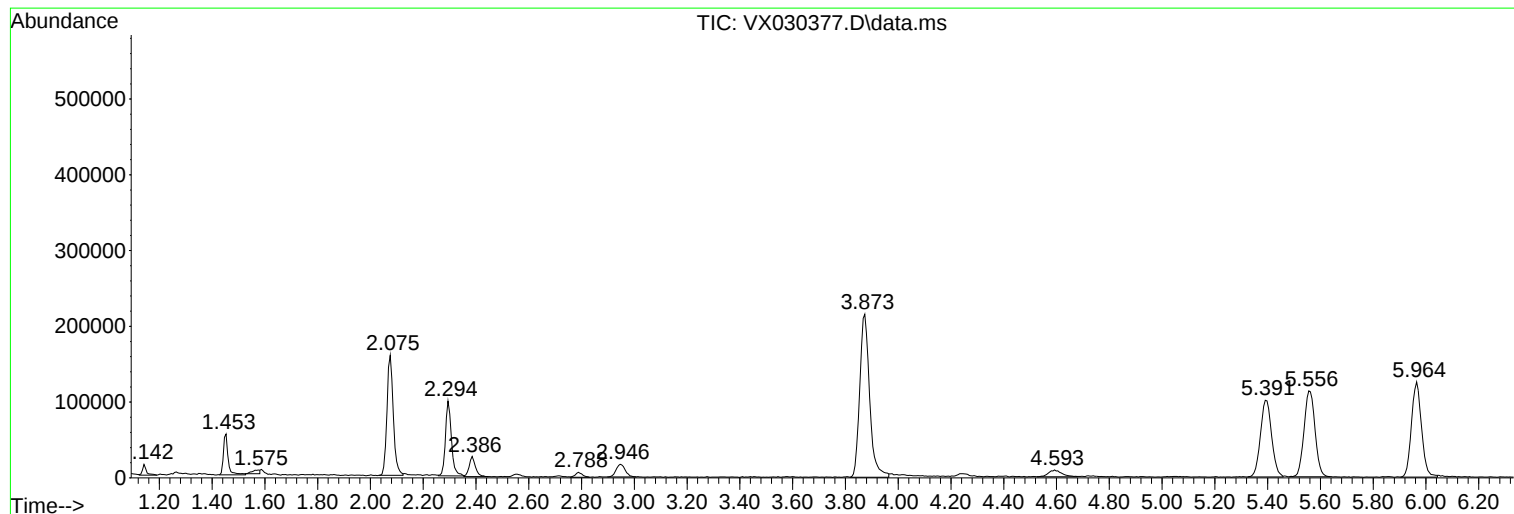
Instrument :
MSVOA_X
ClientSampleId :
33773-74

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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



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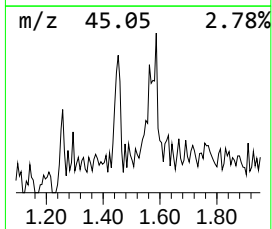
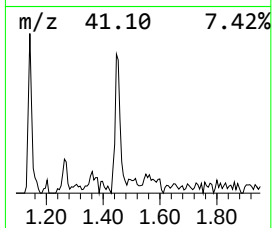
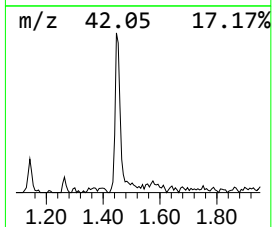
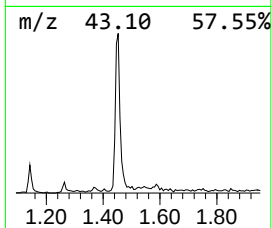
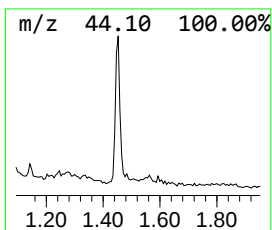
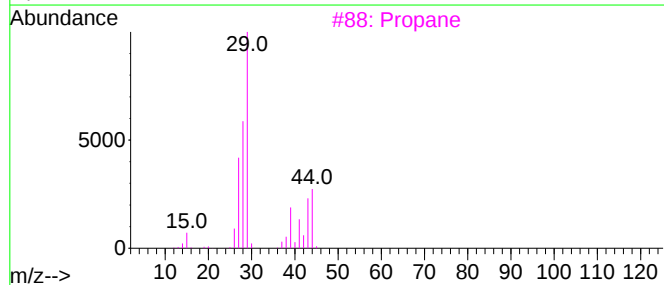
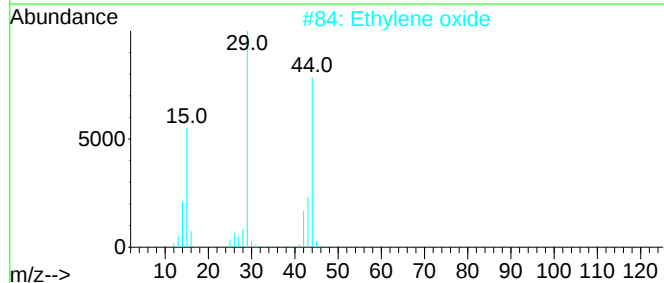
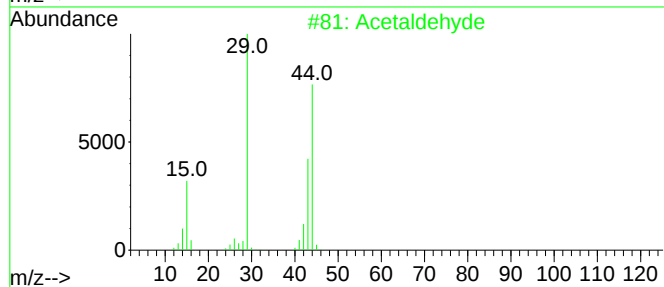
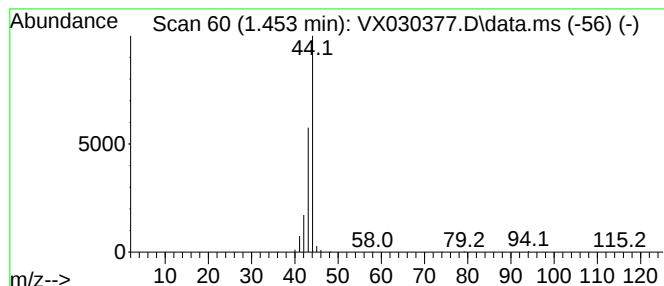
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	10.16 ug/l	66865	Pentafluorobenzene	5.556

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			2-Hexanamine, 4-methyl-	115	C7H17N	000105-41-9	5
5			Tuaminoheptane	115	C7H17N	000123-82-0	5



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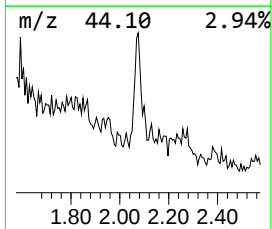
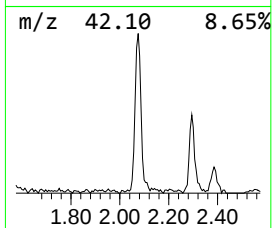
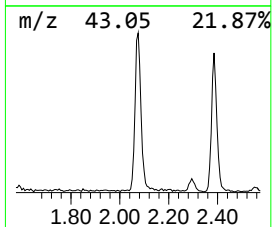
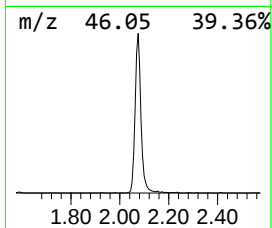
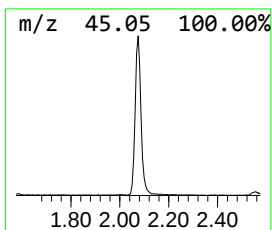
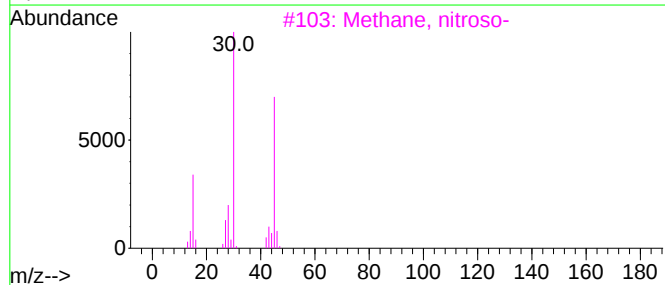
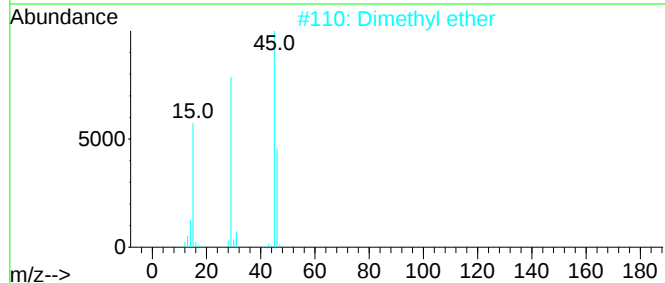
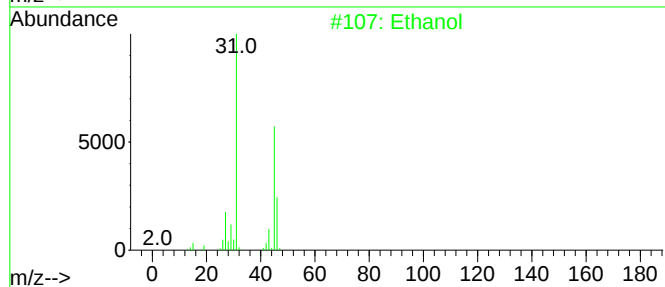
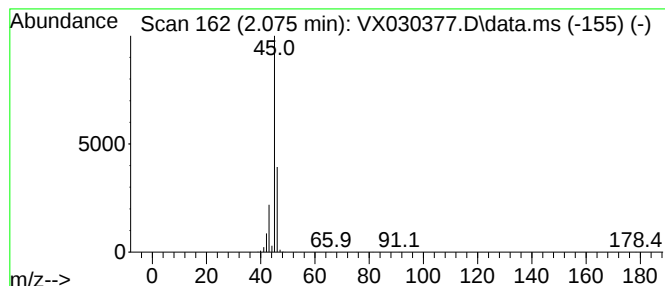
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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.
2.075	39.88 ug/l	262413	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
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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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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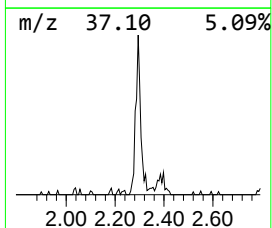
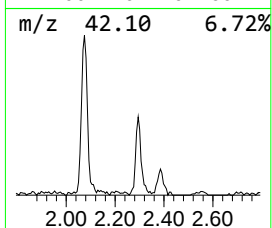
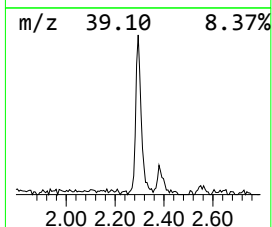
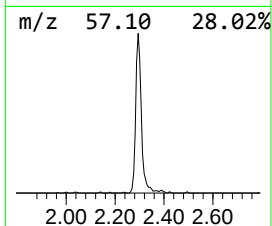
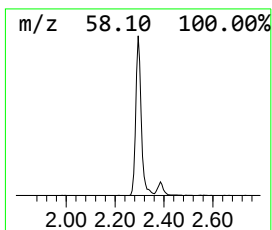
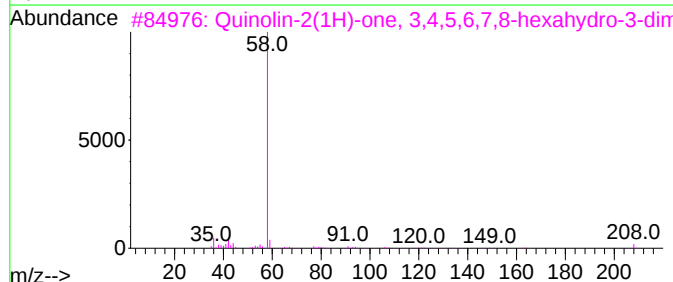
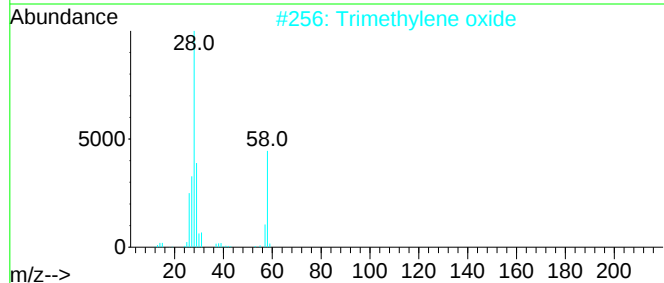
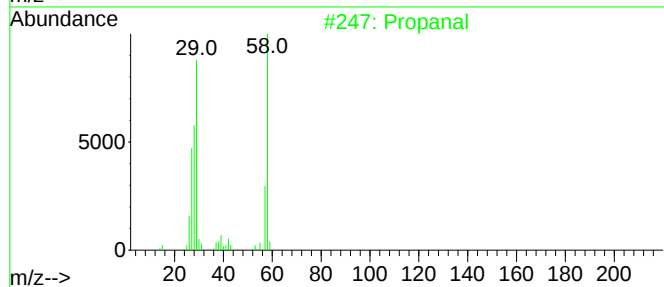
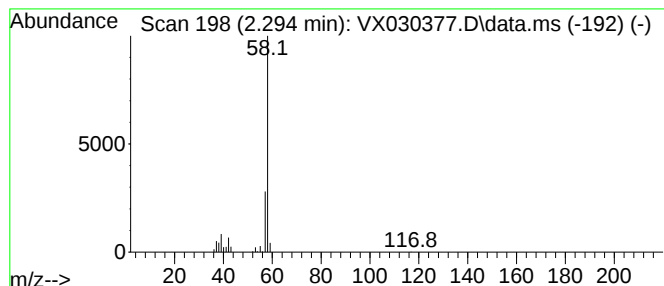
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Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	23.29 ug/l	153267	Pentafluorobenzene	5.556

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		Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
5		Propylene oxide	58	C3H6O	000075-56-9	7



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ALS Vial : 18 Sample Multiplier: 1

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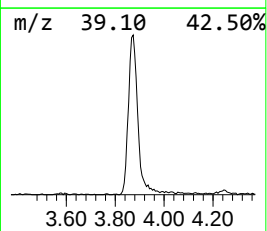
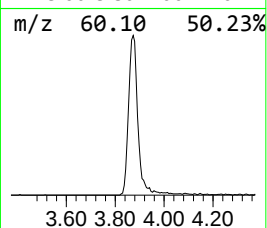
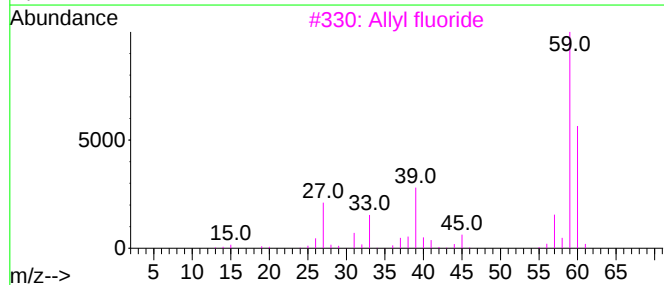
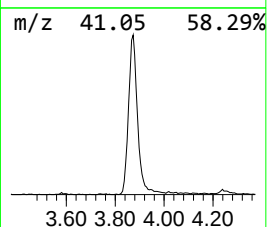
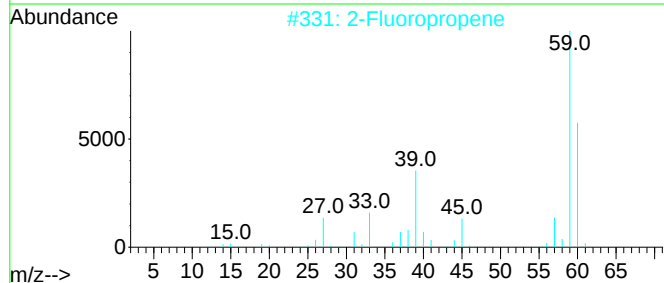
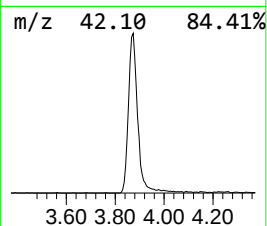
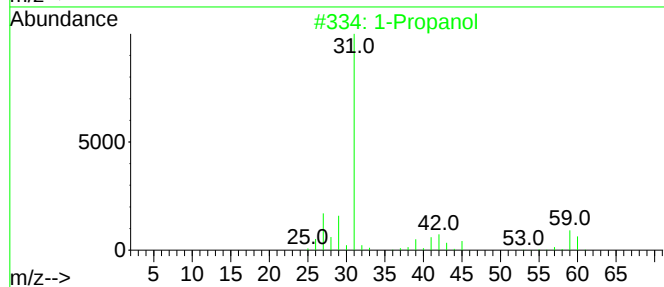
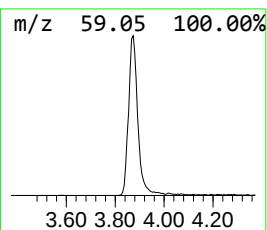
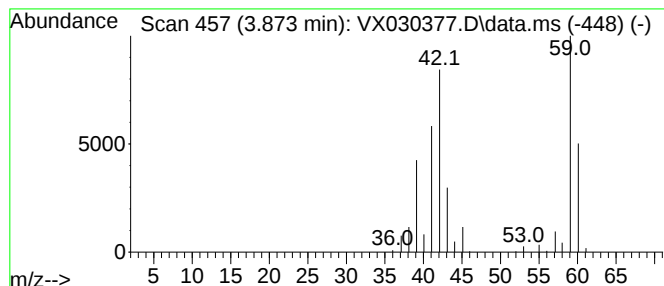
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Quant Title : SW846 8260

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

Peak Number 4 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.873	85.47 ug/l	562349	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	59
2	2-Fluoropropene			60	C3H5F	001184-60-7	52
3	Allyl fluoride			60	C3H5F	000818-92-8	35
4	Cyclopropane			42	C3H6	000075-19-4	25
5	2-Butanol, 3-methoxy-			104	C5H12O2	053778-72-6	10



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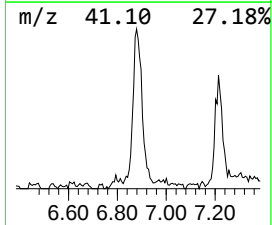
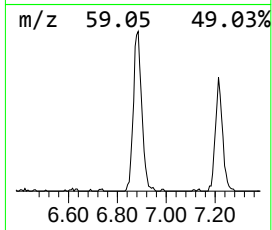
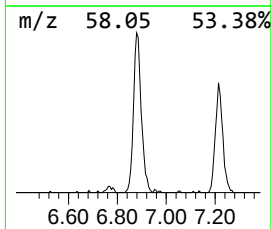
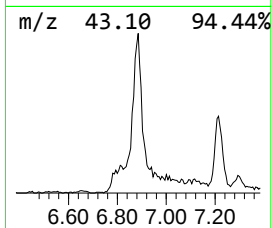
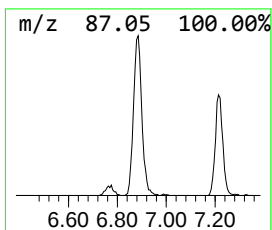
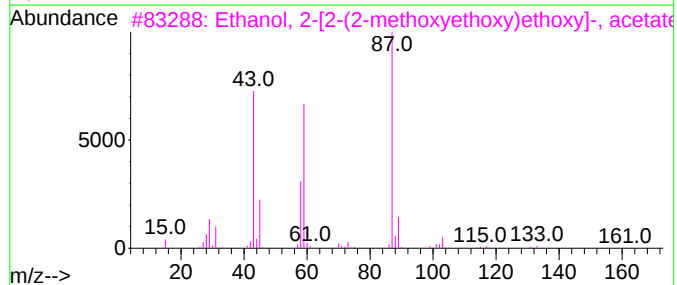
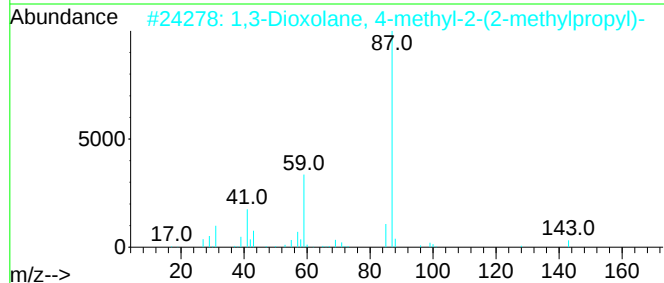
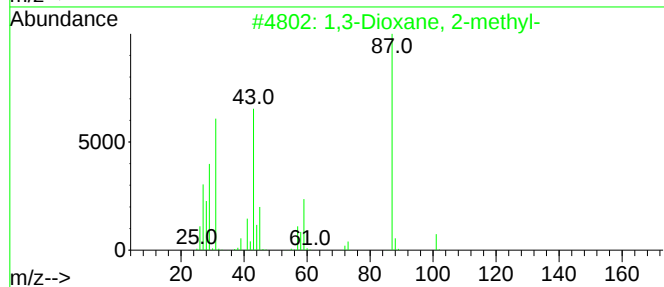
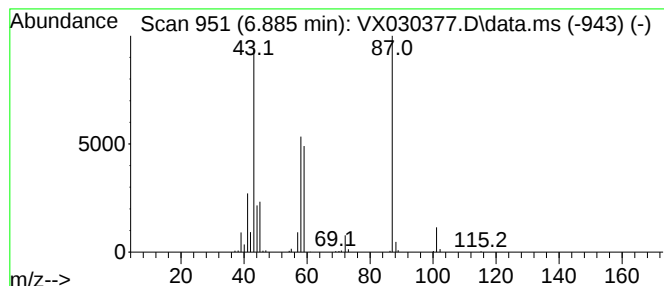
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Quant Title : SW846 8260

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

Peak Number 5 1,3-Dioxane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.885	17.30 ug/l	163501	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	53
2			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	37
3			Ethanol, 2-[2-(2-methoxyethoxy)e...	206	C9H18O5	003610-27-3	36
4			Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	36
5			Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	32



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33773-74

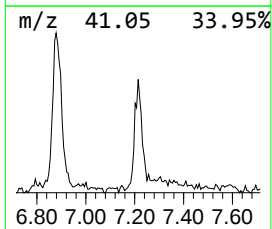
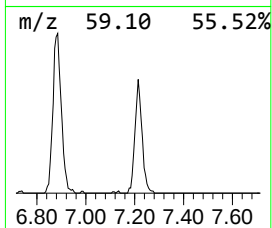
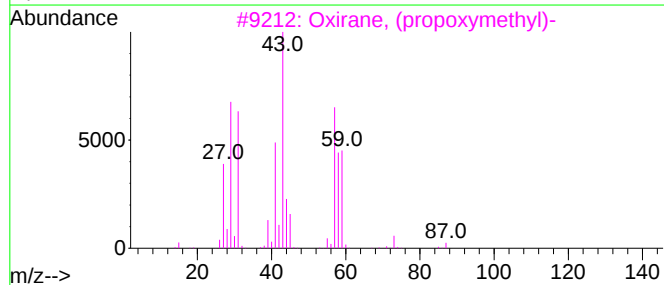
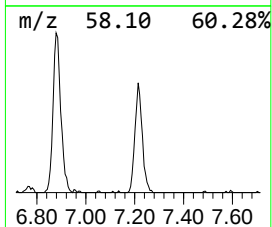
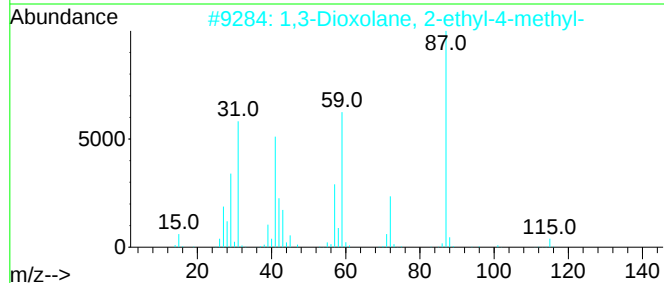
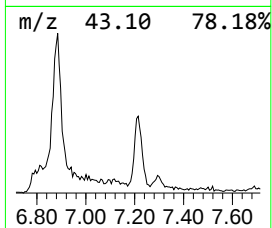
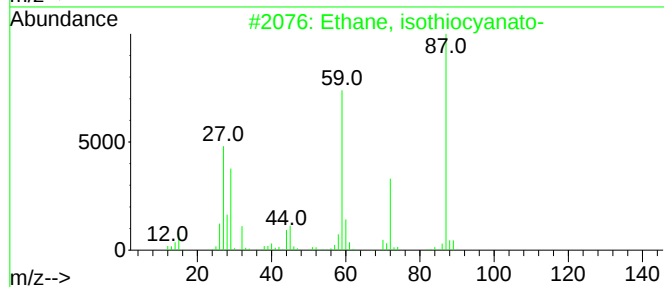
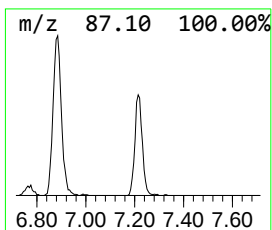
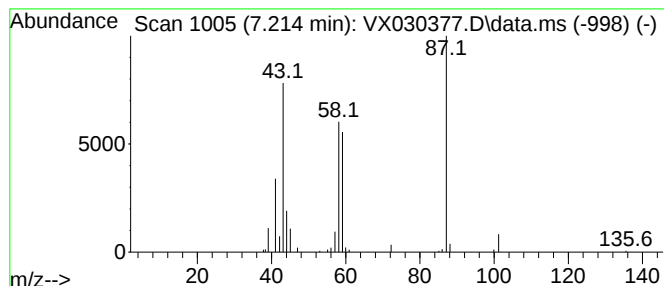
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Quant Title : SW846 8260

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

Peak Number 6 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	8.27 ug/l	78203	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	40
2			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	38
3			Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	38
4			Oxirane, tetramethyl-	100	C6H12O	005076-20-0	14
5			N,N-Dimethylformamide-di-t-butyl...	203	C11H25NO2	036805-97-7	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030377.D
Acq On : 03 Aug 2022 17:44
Operator : JC/MD
Sample : N4018-03 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
33773-74

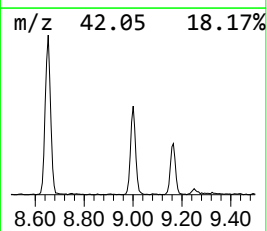
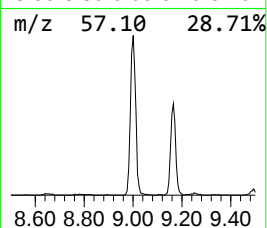
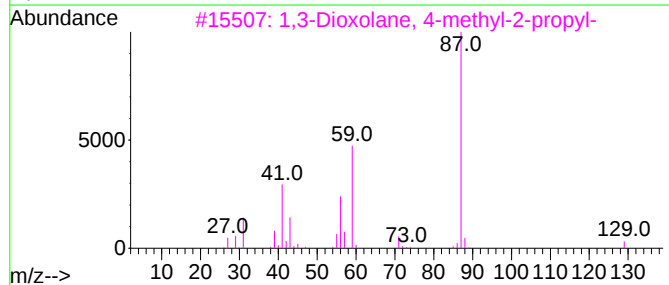
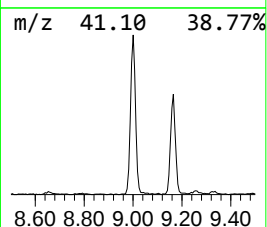
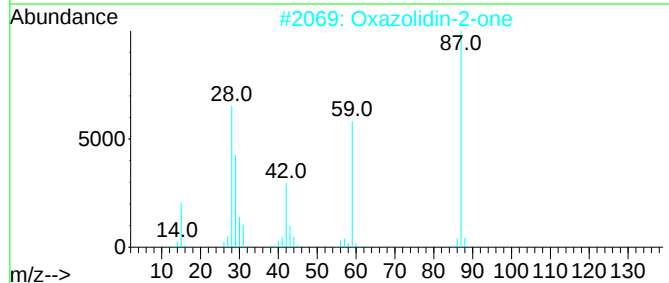
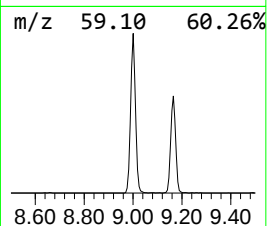
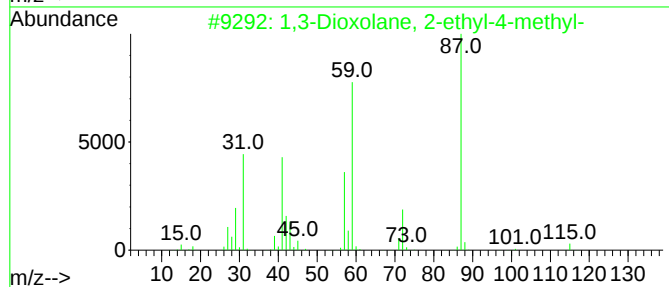
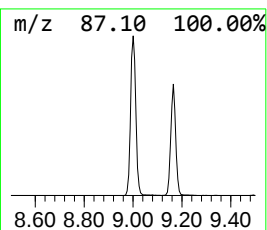
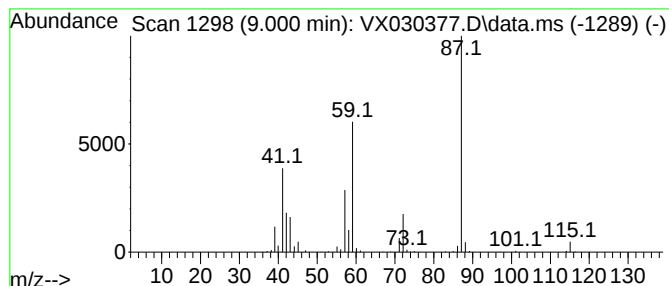
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Quant Title : SW846 8260

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

Peak Number 7 Oxazolidin-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.000	37.70 ug/l	429593	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	90
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
3			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	59
4			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030377.D
Acq On : 03 Aug 2022 17:44
Operator : JC/MD
Sample : N4018-03 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
33773-74

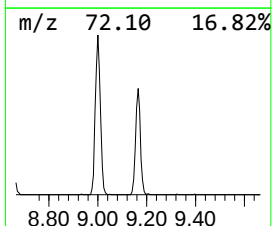
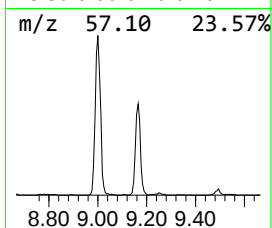
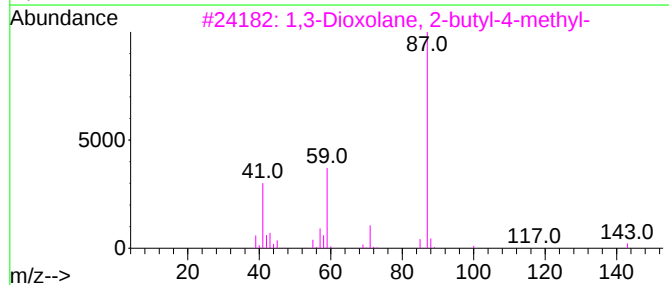
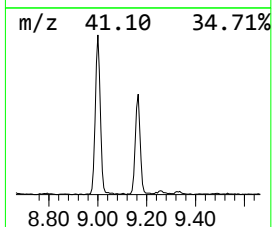
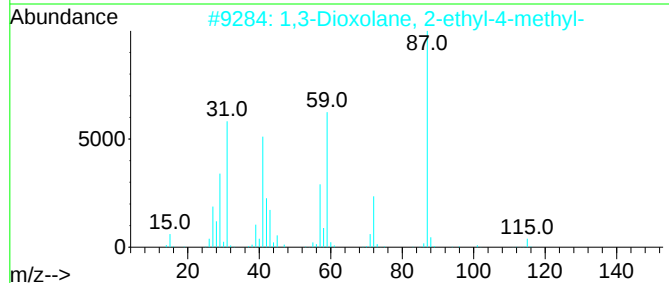
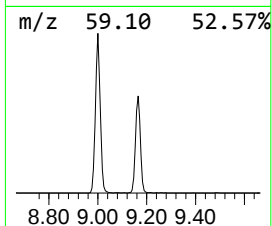
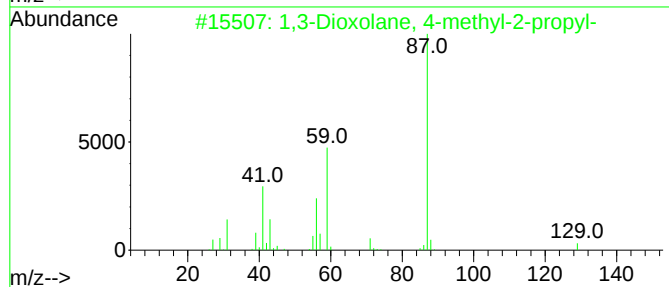
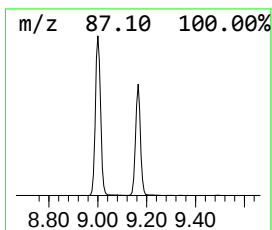
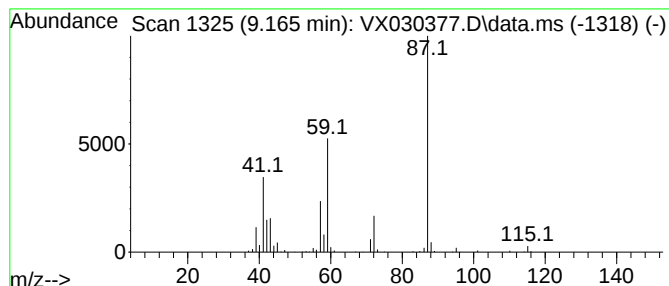
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 8 2-Propanone, O-methyloxime Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.165	23.07 ug/l	262917	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	72
2			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	70
3			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	56
4			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030377.D
Acq On : 03 Aug 2022 17:44
Operator : JC/MD
Sample : N4018-03 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
33773-74

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.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	1.453	10.2	ug/l	66865	1	5.556	328993	50.0
Ethanol	2.075	39.9	ug/l	262413	1	5.556	328993	50.0
Propanal	2.294	23.3	ug/l	153267	1	5.556	328993	50.0
1-Propanol	3.873	85.5	ug/l	562349	1	5.556	328993	50.0
1,3-Dioxane, 2-...	6.885	17.3	ug/l	163501	2	6.769	472562	50.0
unknown-01	7.214	8.3	ug/l	78203	2	6.769	472562	50.0
Oxazolidin-2-one	9.000	37.7	ug/l	429593	3	10.055	569808	50.0
2-Propanone, 0-...	9.165	23.1	ug/l	262917	3	10.055	569808	50.0