

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051821\
 Data File : VN067125.D
 Acq On : 18 May 2021 14:28
 Operator : JC/MD
 Sample : M2387-07 20X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41800

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\82N051421W.M

Title : SW846 8260

Signal : TIC: VN067125.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.997	82	96	130	rBV	3877287	6133835	100.00%	21.604%
2	2.305	198	211	234	rBV	457719	767705	12.52%	2.704%
3	3.654	694	714	738	rBV	152541	401925	6.55%	1.416%
4	3.770	739	757	801	rVB	254372	702548	11.45%	2.474%
5	4.016	834	849	875	rVB2	25744	76762	1.25%	0.270%
6	5.961	1546	1574	1624	rBV2	228129	821664	13.40%	2.894%
7	6.763	1847	1873	1914	rBV2	33925	112993	1.84%	0.398%
8	7.522	2131	2156	2169	rBV	475260	1203374	19.62%	4.238%
9	7.597	2170	2184	2218	rVB	833379	2045111	33.34%	7.203%
10	7.959	2297	2319	2351	rBV	467369	1139127	18.57%	4.012%
11	8.528	2508	2531	2572	rBV3	1428955	3202560	52.21%	11.280%
12	8.782	2607	2626	2645	rBV2	163020	347369	5.66%	1.223%
13	10.037	3075	3094	3134	rBV	1949476	3726735	60.76%	13.126%
14	11.357	3569	3586	3636	rBV	1429296	2739362	44.66%	9.648%
15	12.357	3943	3959	4009	rBV	1120413	2327328	37.94%	8.197%
16	13.299	4295	4310	4344	rBV	1382836	2643220	43.09%	9.310%

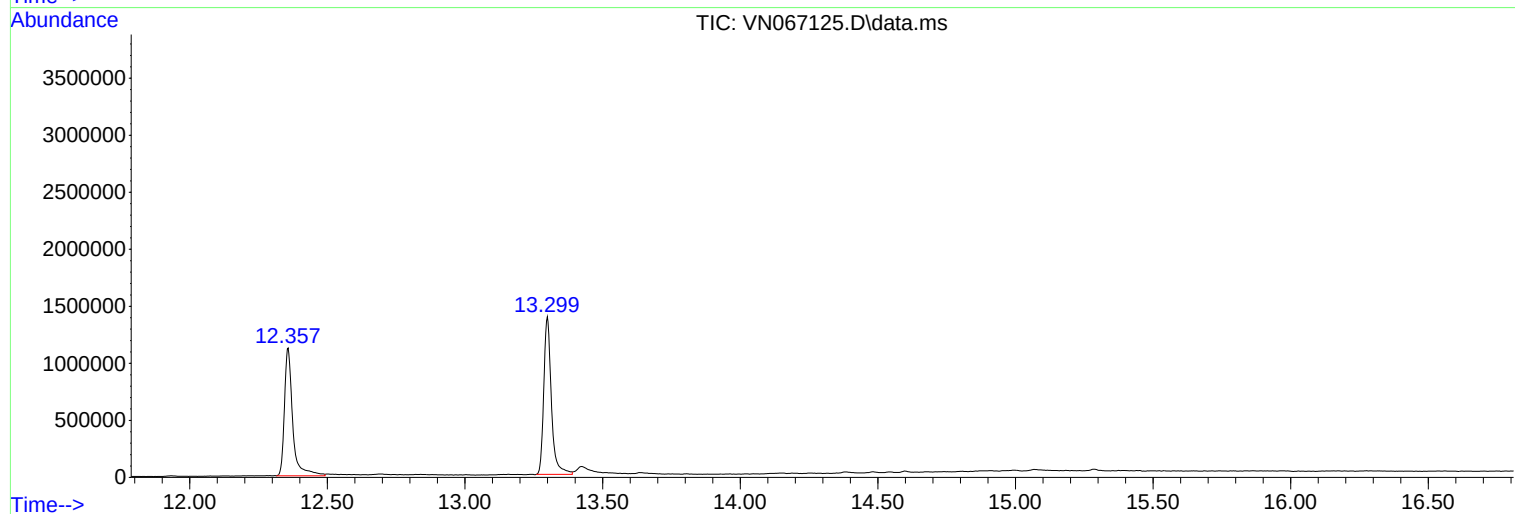
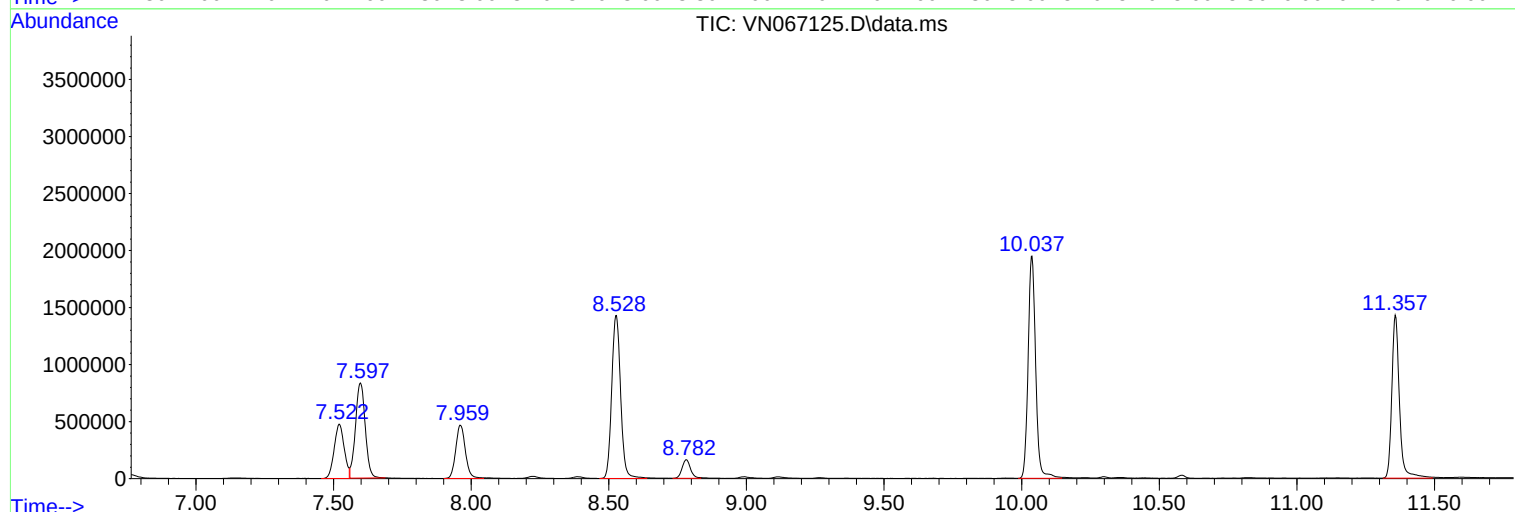
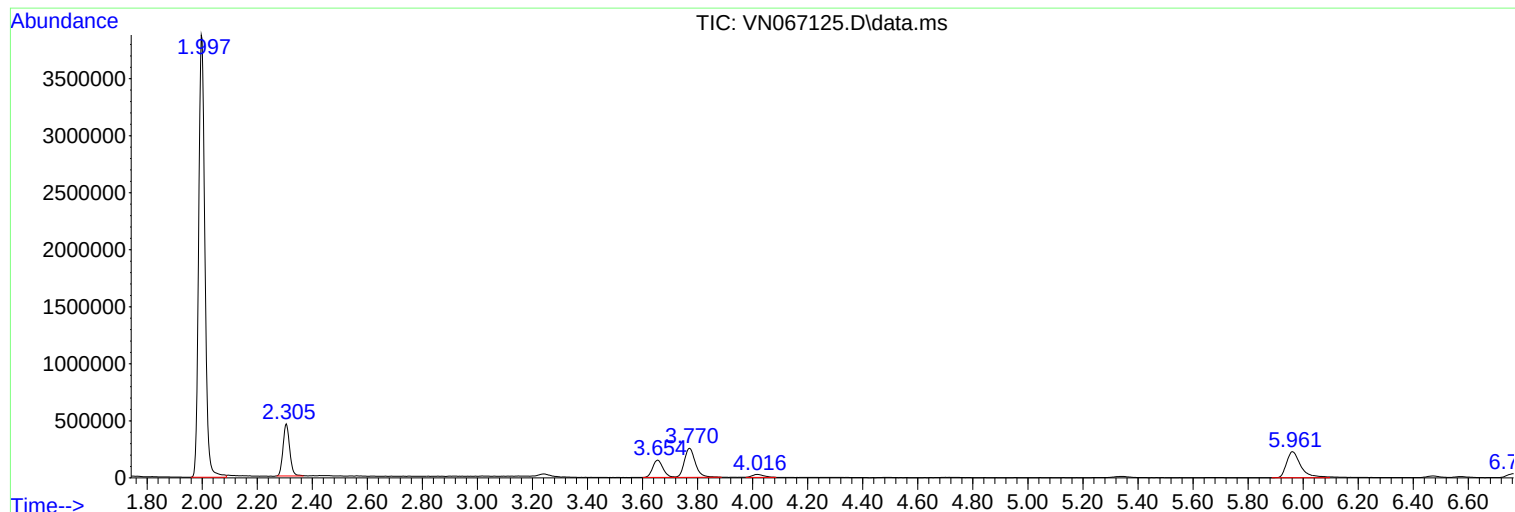
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
41800

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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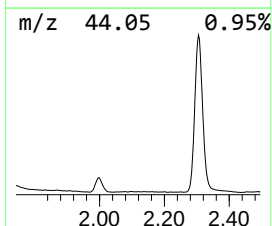
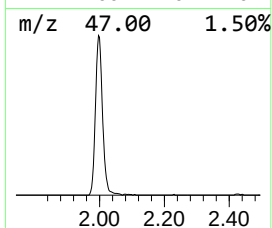
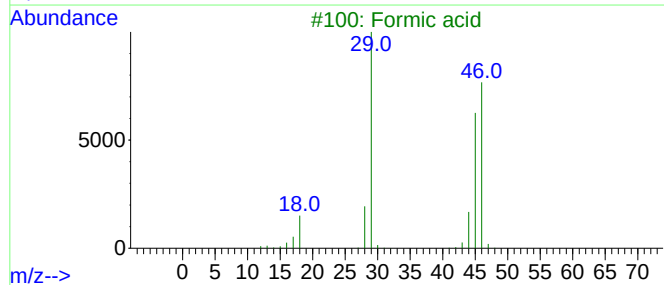
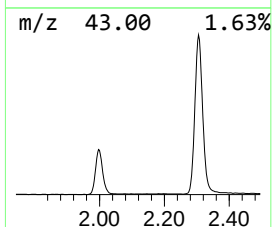
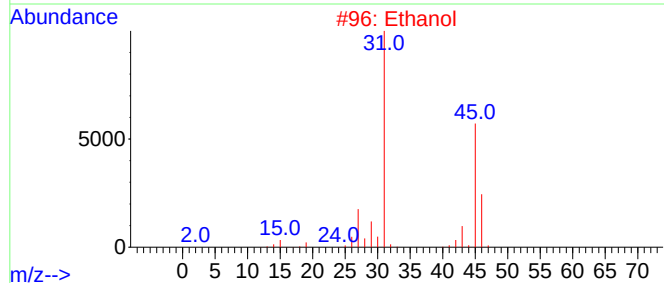
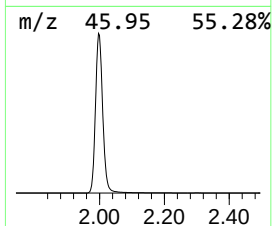
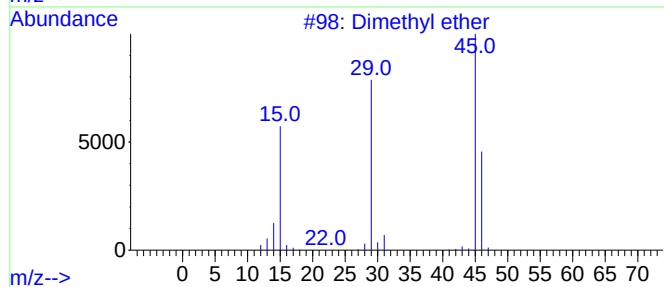
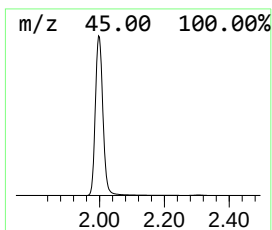
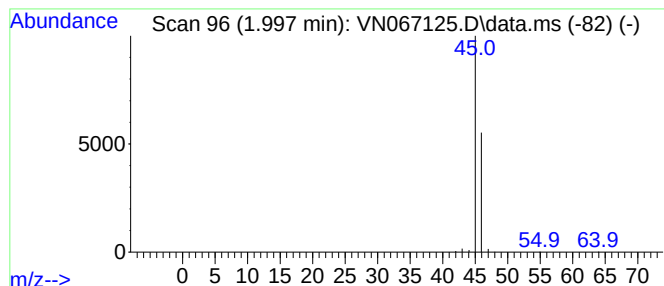
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Dimethyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.997	149.96 ug/l	6133840	Pentafluorobenzene	7.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	90
2			Ethanol	46	C2H6O	000064-17-5	7
3			Formic acid	46	CH2O2	000064-18-6	7
4			Hydrazine, methyl-	46	CH6N2	000060-34-4	4
5			Ethene, fluoro-	46	C2H3F	000075-02-5	4



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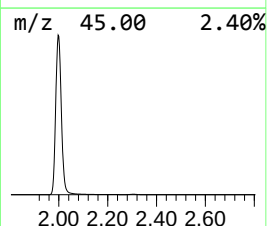
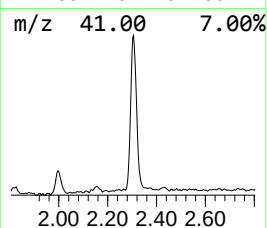
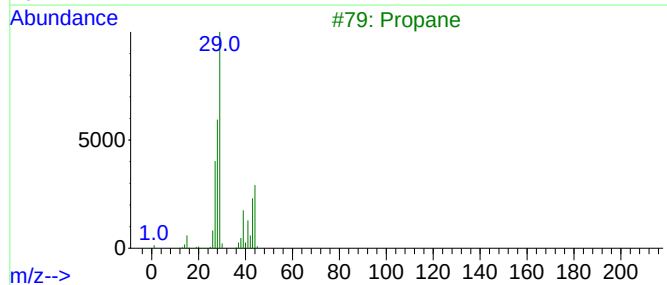
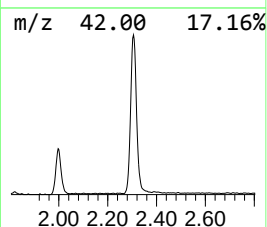
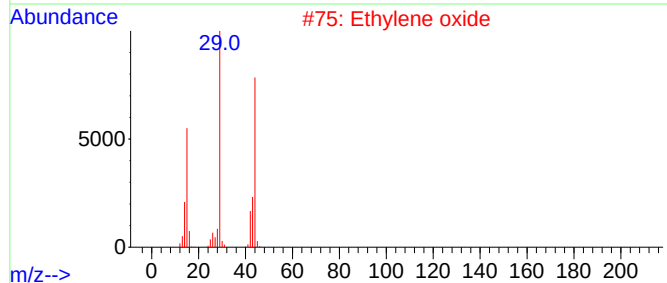
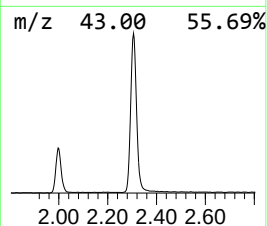
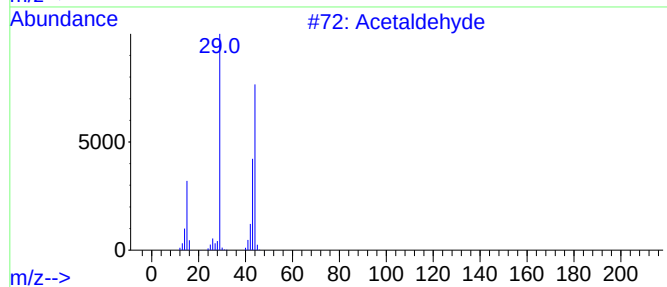
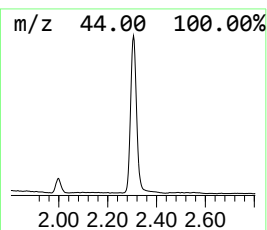
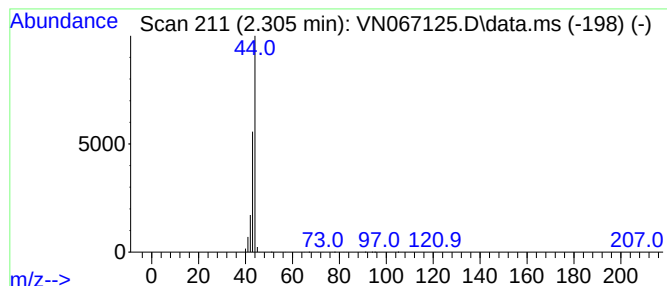
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.305	18.77 ug/l	767705	Pentafluorobenzene	7.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Ethyne, fluoro-	44	C2HF	002713-09-9	3



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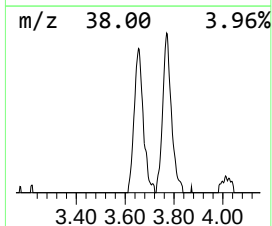
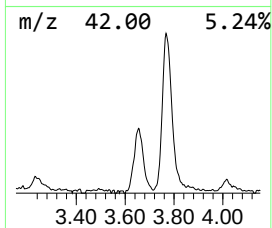
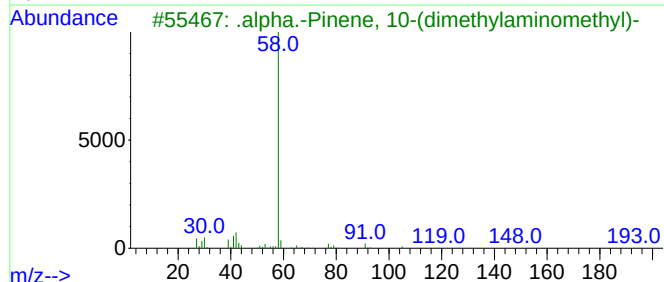
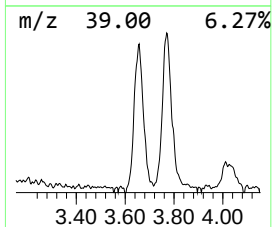
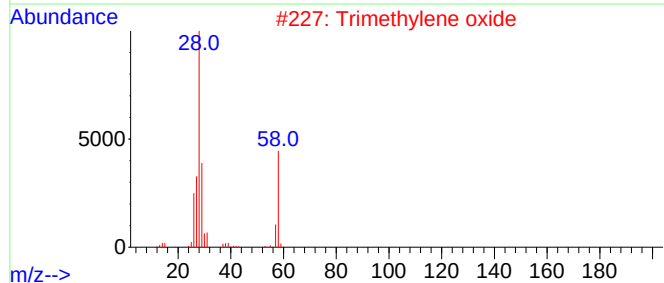
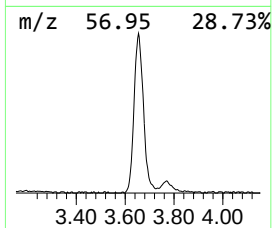
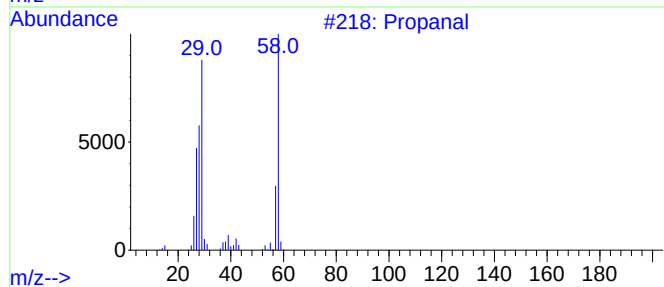
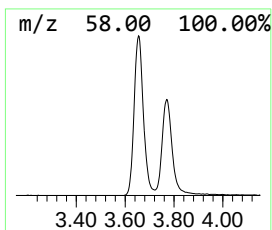
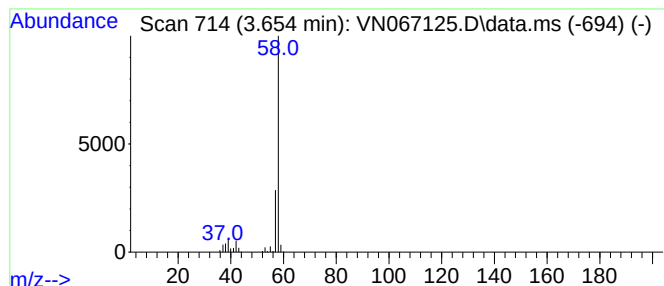
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.654	9.83 ug/l	401925	Pentafluorobenzene	7.597

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			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
4			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
5			Propylene oxide	58	C3H6O	000075-56-9	7



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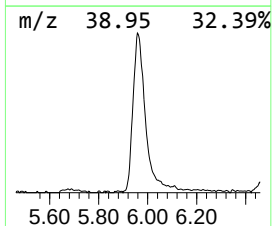
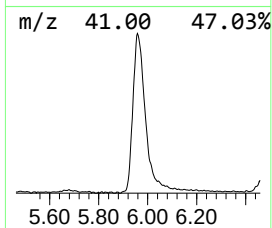
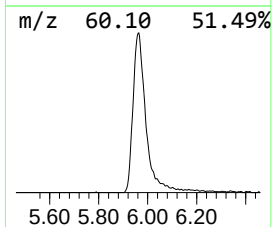
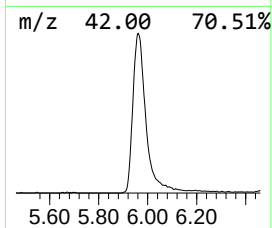
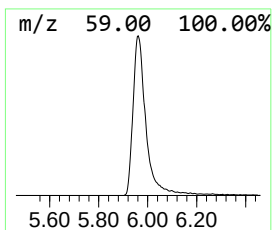
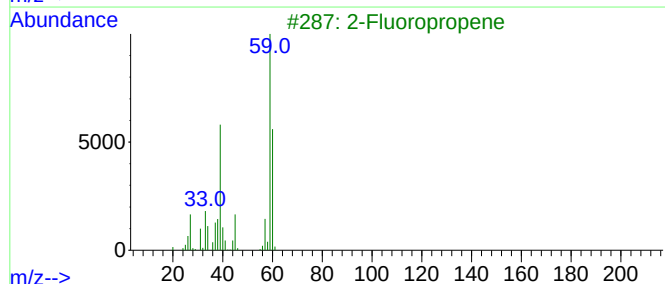
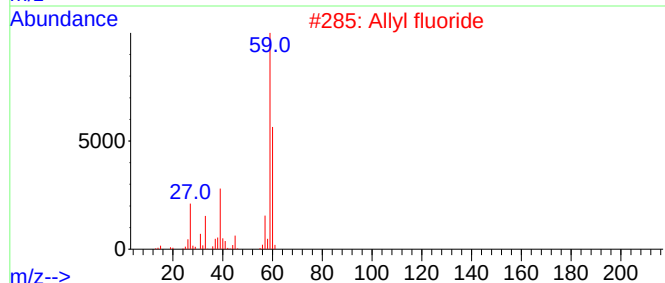
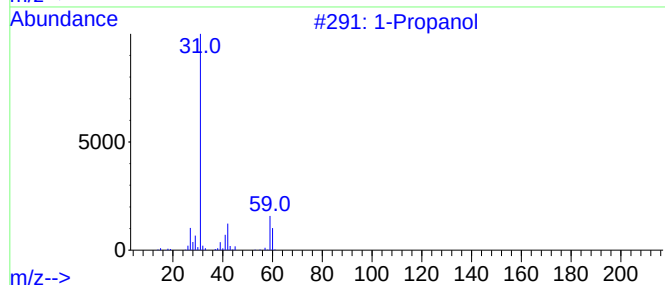
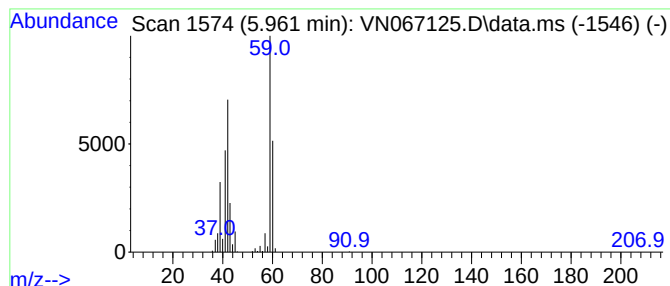
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.961	20.09 ug/l	821664	Pentafluorobenzene	7.597

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	78
2		Allyl fluoride	60	C3H5F	000818-92-8	42
3		2-Fluoropropene	60	C3H5F	001184-60-7	38
4		5-Hexyn-3-ol	98	C6H10O	019780-84-8	23
5		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	17



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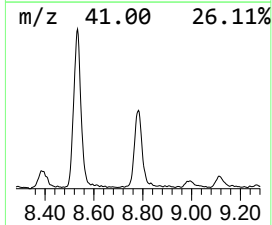
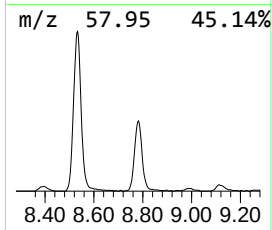
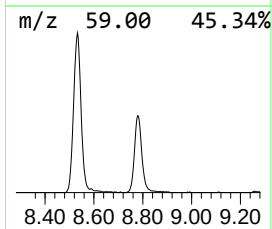
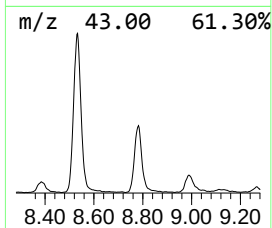
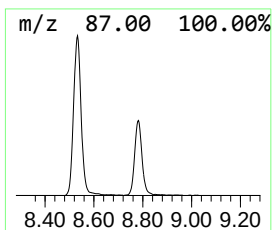
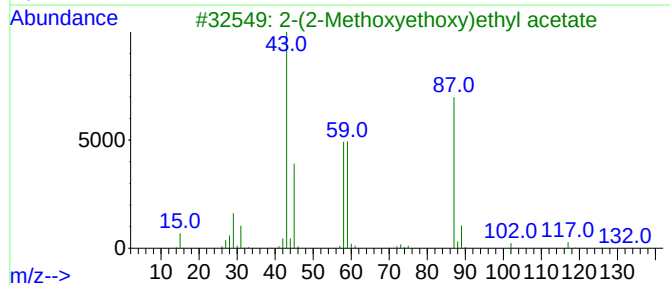
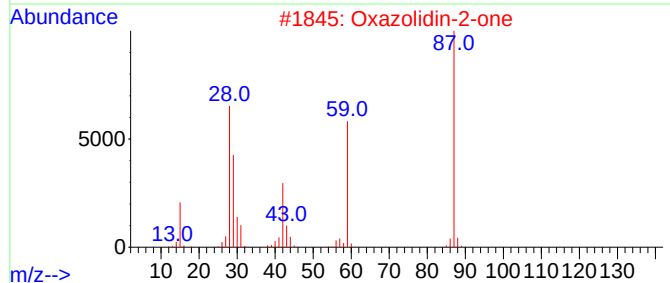
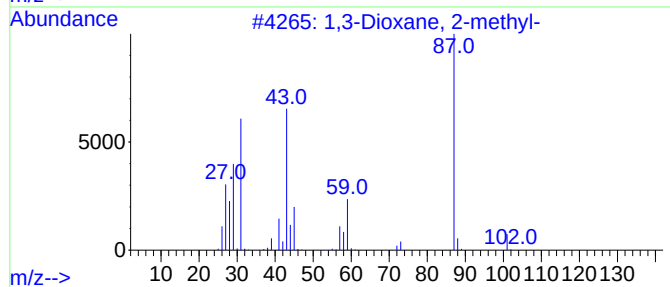
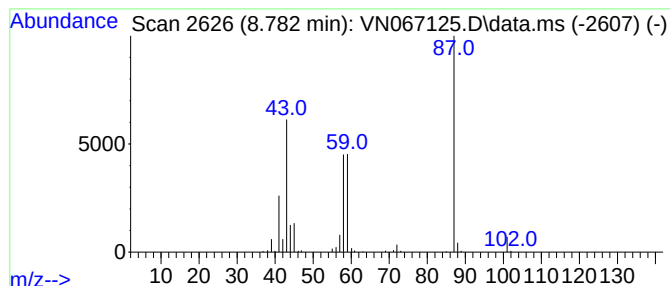
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.782	5.42 ug/l	347369	1,4-Difluorobenzene	8.525

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	52
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	50
3			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
4			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	36
5			Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl ether	1.997	150.0	ug/l	6133840	1	7.597	2045110	50.0
Acetaldehyde	2.305	18.8	ug/l	767705	1	7.597	2045110	50.0
Propanal	3.654	9.8	ug/l	401925	1	7.597	2045110	50.0
1-Propanol	5.961	20.1	ug/l	821664	1	7.597	2045110	50.0
1,3-Dioxane, 2-...	8.782	5.4	ug/l	347369	2	8.525	3202560	50.0