

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
 Data File : VN069122.D
 Acq On : 22 Oct 2021 6:18
 Operator : JC/MD
 Sample : M4284-15
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 30848

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\82N101221W.M

Title : SW846 8260

Signal : TIC: VN069122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.564	198	214	268	rBV	6782435	15285498	3.59%	2.230%
2	4.167	753	812	1043	rBV5	29226708	425257344	100.00%	62.053%
3	6.734	1686	1769	1823	rVV	16675639	113631453	26.72%	16.581%
4	9.561	2804	2823	2870	rVB2	17433490	38959157	9.16%	5.685%
5	10.443	3129	3152	3170	rBV	2347666	4514114	1.06%	0.659%
6	10.607	3183	3213	3231	rVV2	2346395	5043976	1.19%	0.736%
7	11.151	3405	3416	3446	rVV	4047443	7019769	1.65%	1.024%
8	11.714	3612	3626	3661	rVB	33318862	70456656	16.57%	10.281%
9	12.739	3995	4008	4041	rVB3	2281606	5146406	1.21%	0.751%

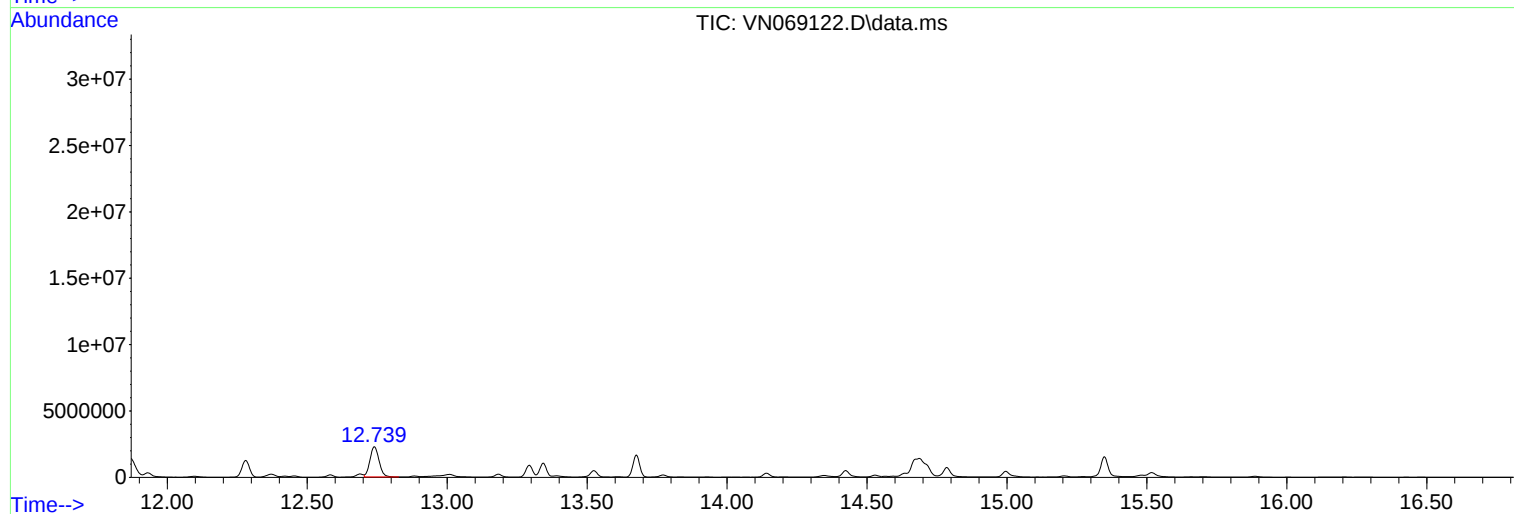
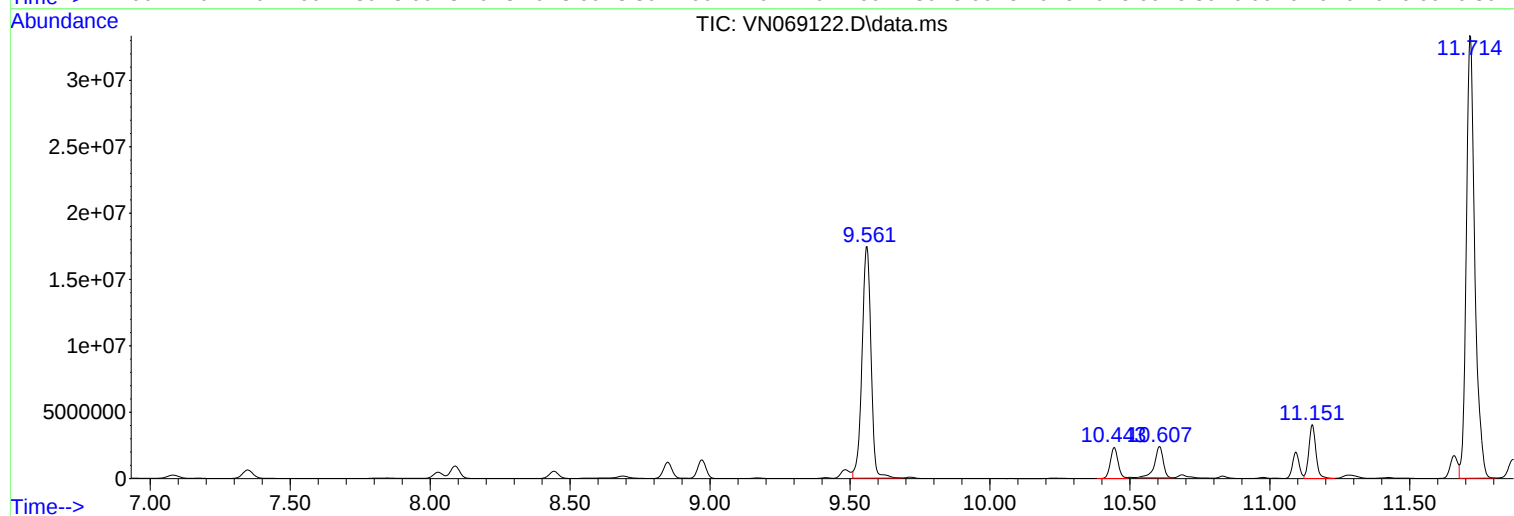
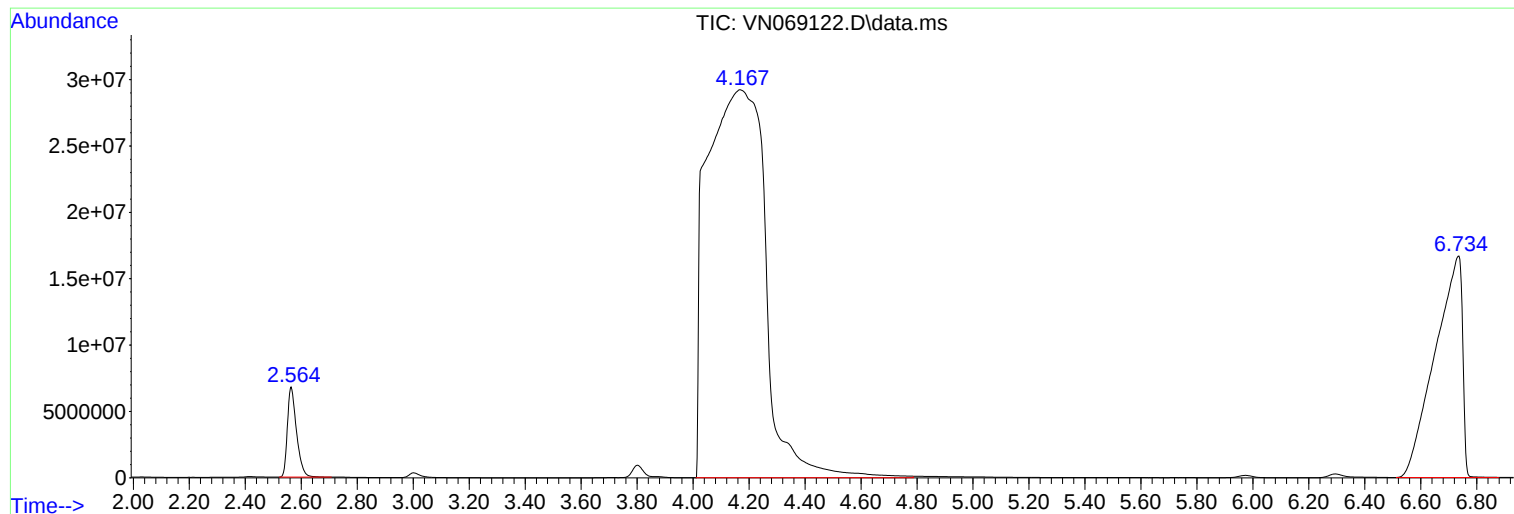
Sum of corrected areas: 685314373

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Quant Title : SW846 8260

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



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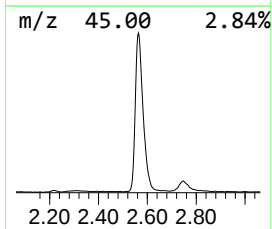
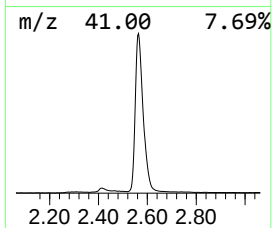
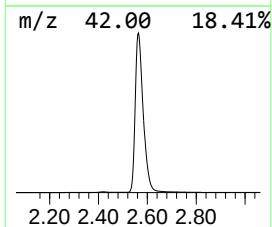
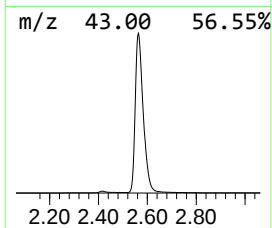
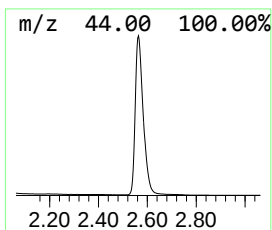
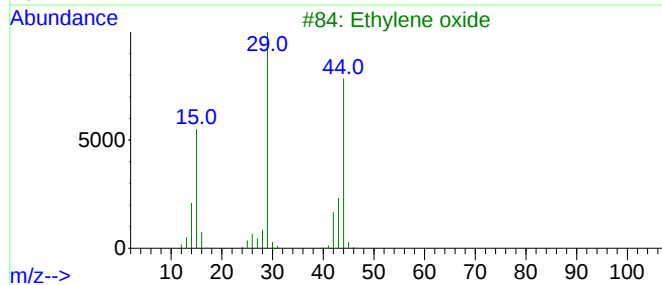
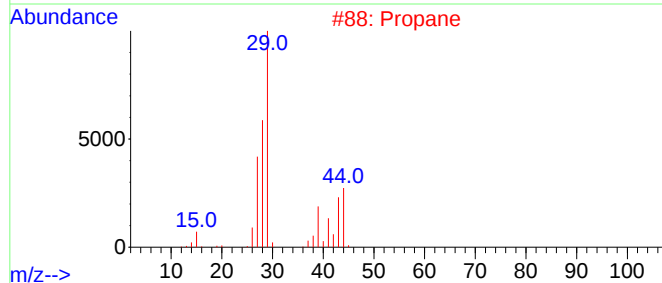
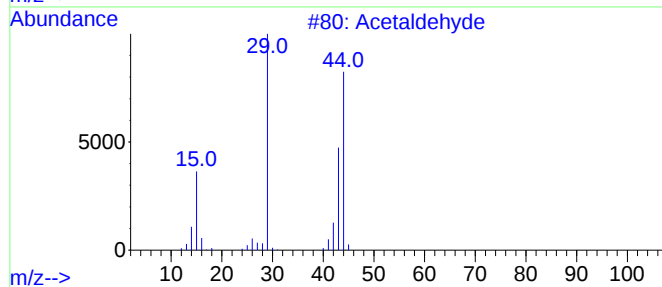
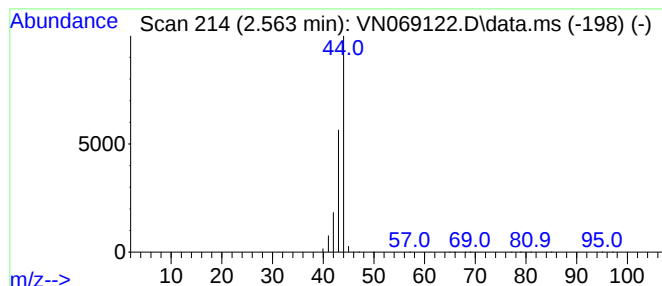
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.563	6.73 ug/l	15285500	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
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			1,2-Propanediamine	74	C3H10N2	000078-90-0	4



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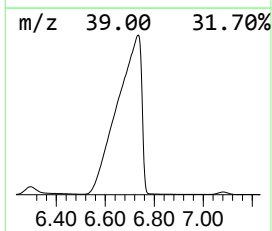
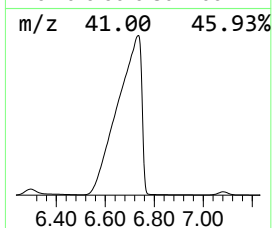
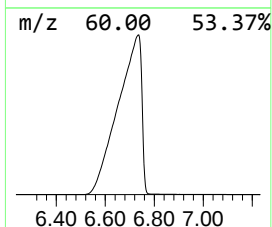
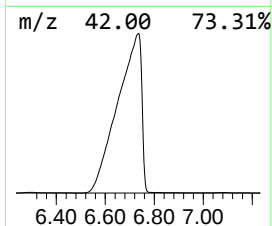
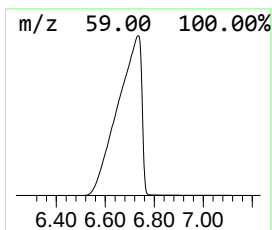
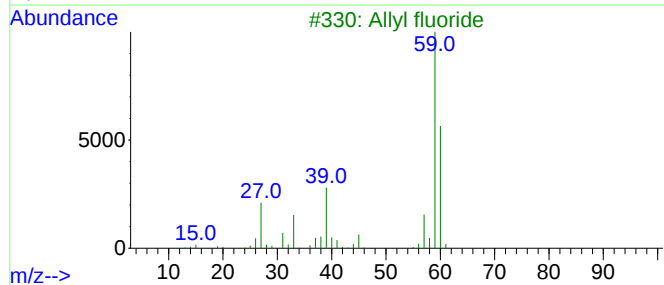
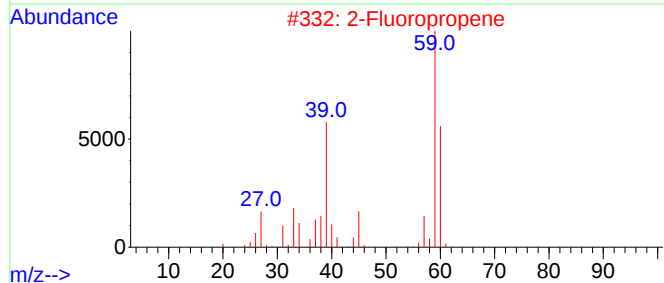
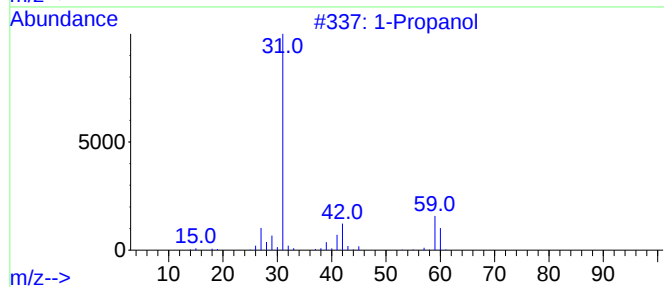
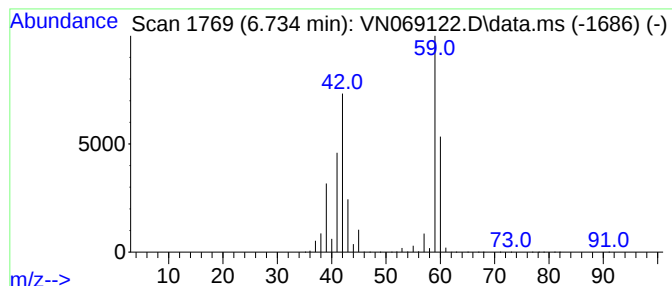
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Peak Number 3 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.734	50.00 ug/l	113631000	Pentafluorobenzene	8.088

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	78
2		2-Fluoropropene	60	C3H5F	001184-60-7	43
3		Allyl fluoride	60	C3H5F	000818-92-8	38
4		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9
5		Acetaldoxime	59	C2H5NO	000107-29-9	7



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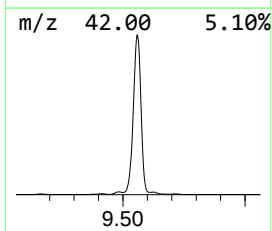
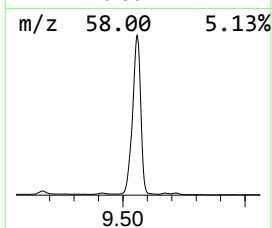
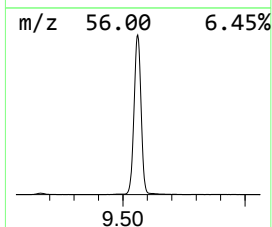
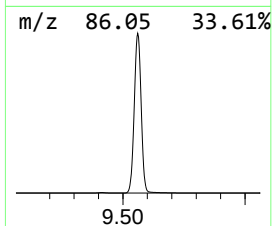
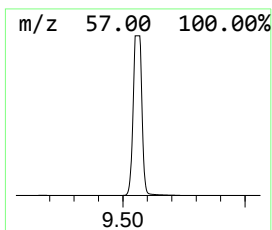
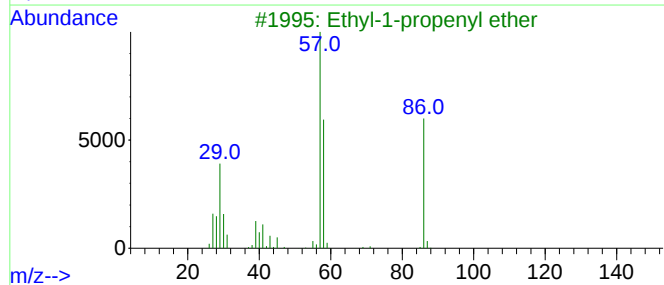
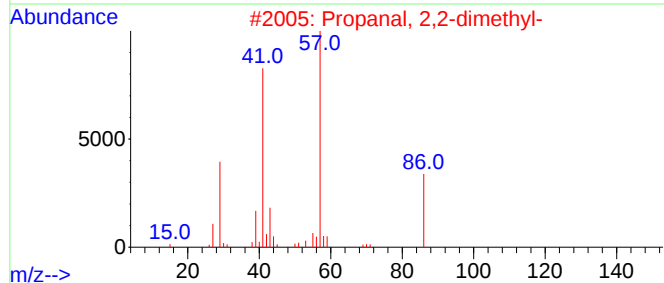
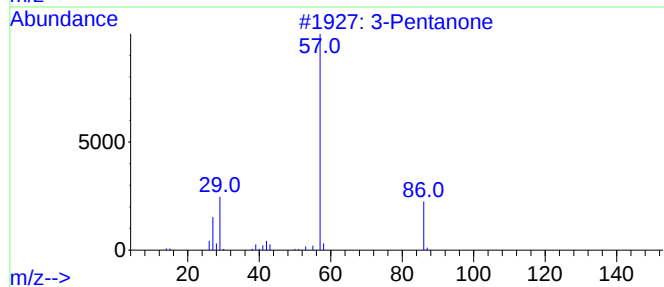
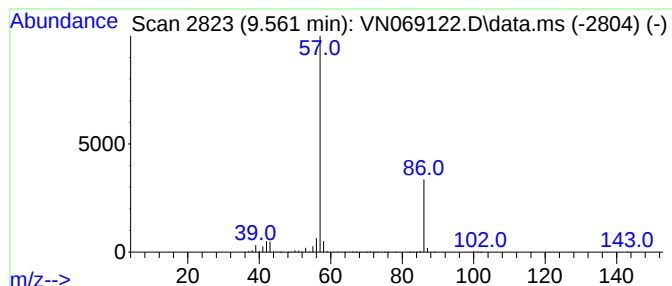
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Peak Number 4 3-Pentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.561	50.00 ug/l	38959200	1,4-Difluorobenzene	8.971

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone	86	C5H10O	000096-22-0	72
2			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	39
3			Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	9
4			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
5			3-Heptanone, 5-ethyl-4-methyl-	156	C10H20O	027607-63-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.563	6.7	ug/l	15285500	1	8.088	113631000	50.0
1-Propanol	6.734	50.0	ug/l	113631000	1	8.088	113631000	50.0
3-Pentanone	9.561	50.0	ug/l	38959200	2	8.971	38959200	50.0