

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062922\
 Data File : VN073247.D
 Acq On : 29 Jun 2022 16:54
 Operator : JC\MD
 Sample : N3504-06 50X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TRE-1618

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\82N062822W.M

Title : SW846 8260

Signal : TIC: VN073247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.546	105	112	141	rBV	6441405	12149014	30.21%	19.103%
2	3.681	285	305	344	rBV	10409368	40218377	100.00%	63.240%
3	4.222	389	397	411	rBV	181985	511122	1.27%	0.804%
4	5.287	563	578	591	rBV2	148096	514490	1.28%	0.809%
5	7.339	918	927	945	rVB	195834	497686	1.24%	0.783%
6	7.951	1021	1031	1036	rBV	237437	570191	1.42%	0.897%
7	8.016	1036	1042	1057	rVB	456038	1037558	2.58%	1.631%
8	8.369	1092	1102	1116	rBV	254581	581244	1.45%	0.914%
9	8.898	1184	1192	1211	rVB	629429	1315500	3.27%	2.069%
10	9.086	1216	1224	1243	rBV	204501	431631	1.07%	0.679%
11	10.375	1431	1443	1451	rBV	844505	1575058	3.92%	2.477%
12	11.680	1657	1665	1676	rBV	904985	1557729	3.87%	2.449%
13	12.669	1826	1833	1846	rVB	732677	1201267	2.99%	1.889%
14	13.610	1985	1993	2003	rBV	852133	1435738	3.57%	2.258%

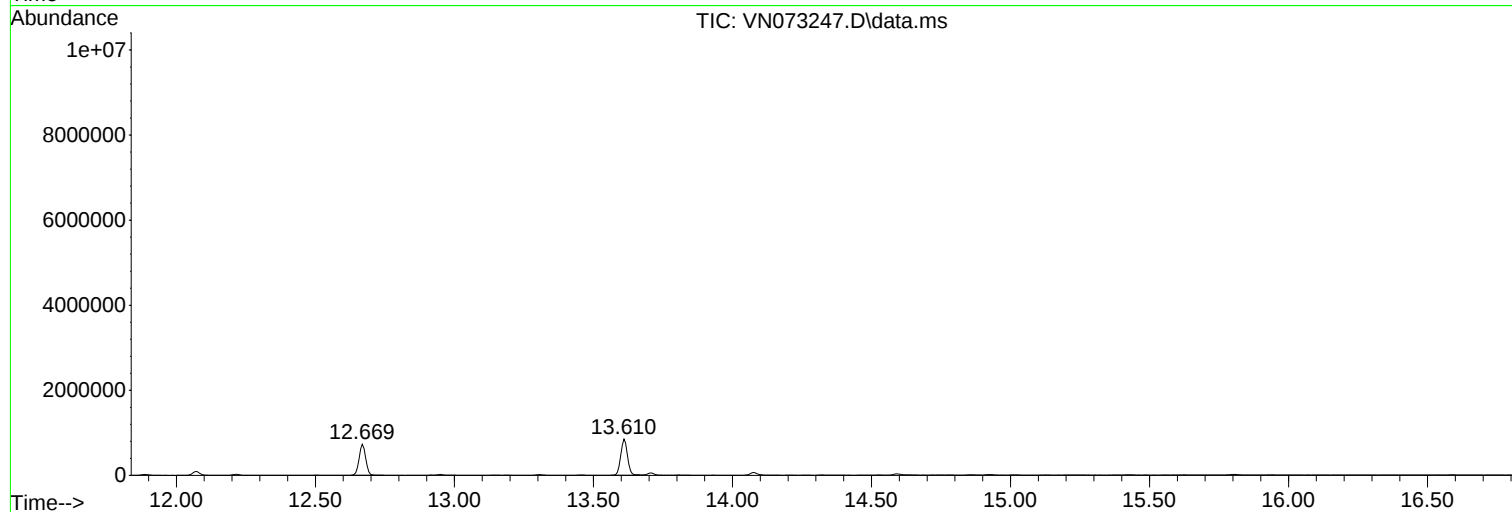
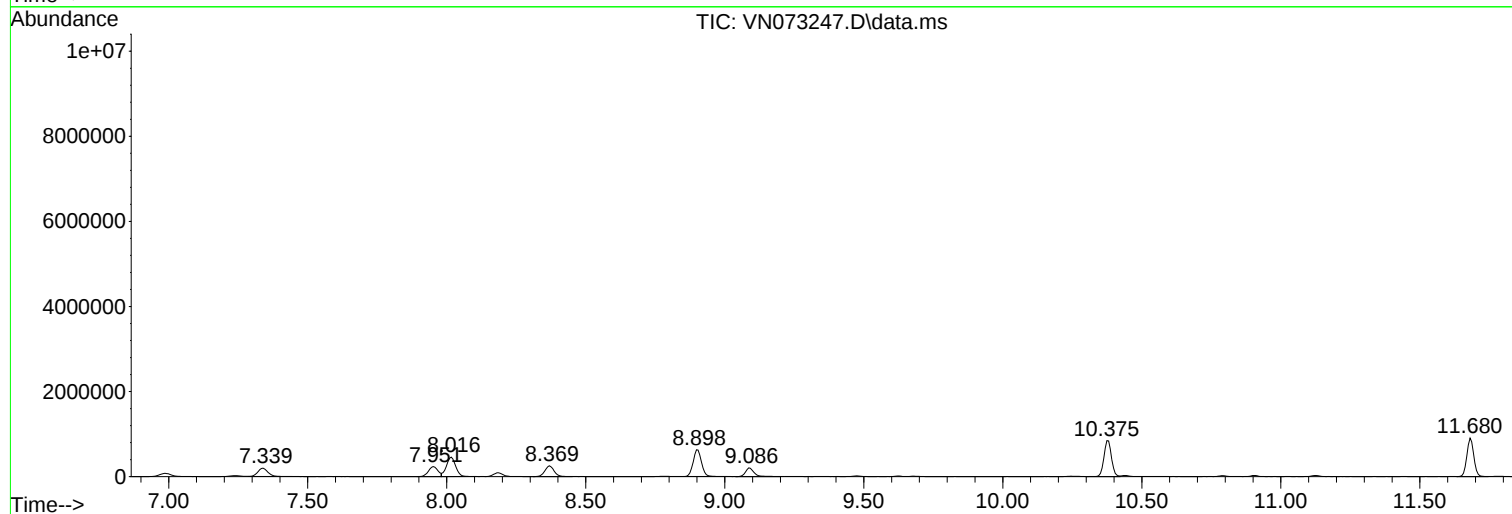
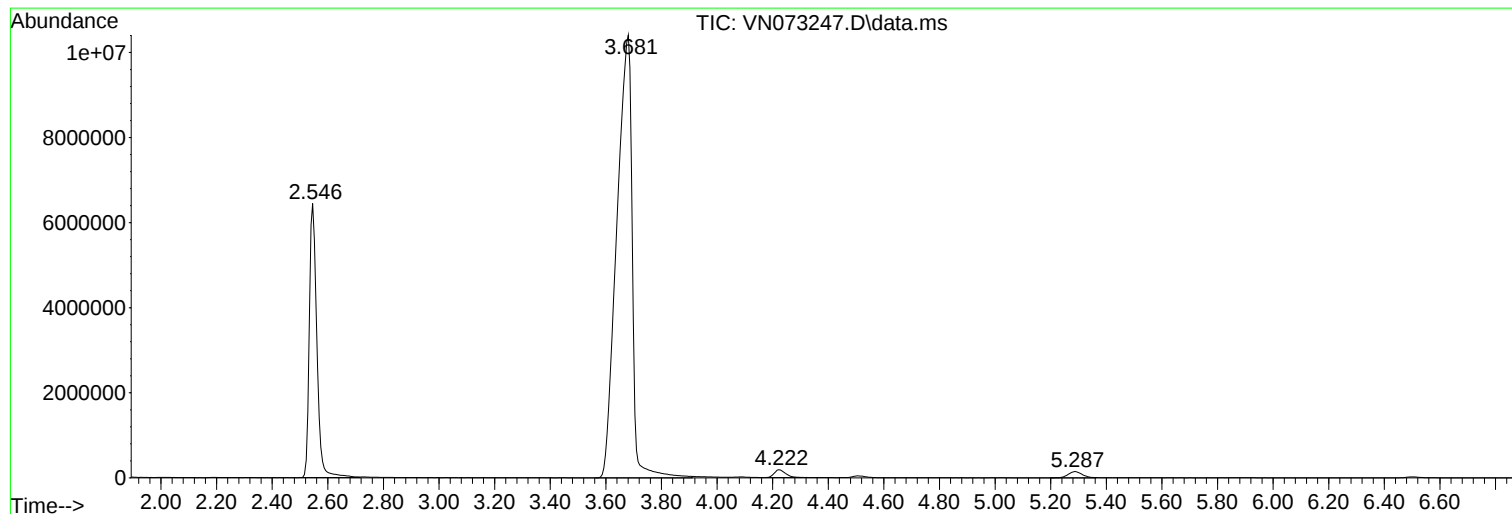
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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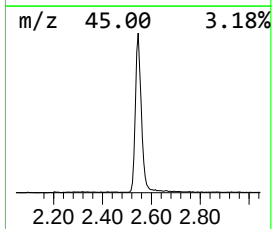
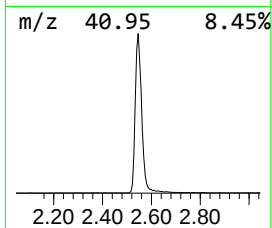
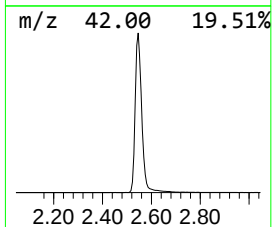
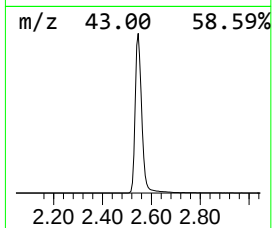
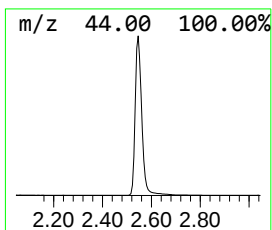
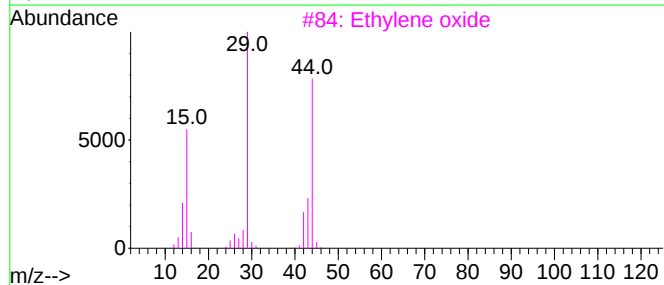
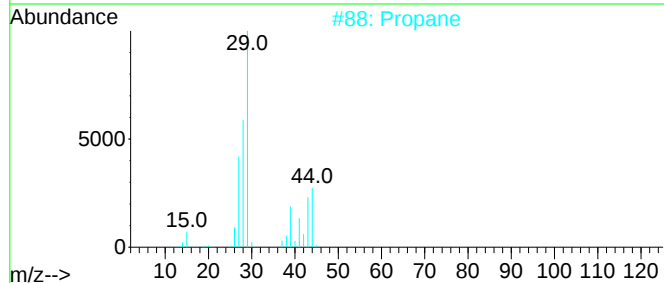
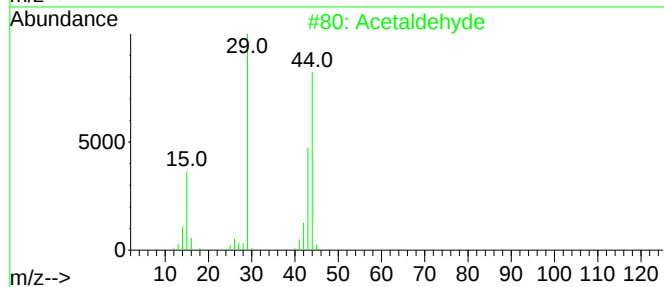
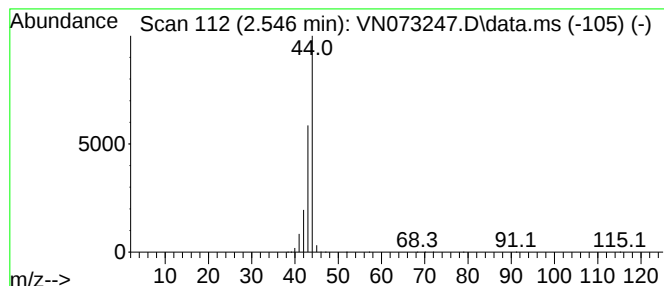
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.546	585.46 ug/l	12149000	Pentafluorobenzene	8.016

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			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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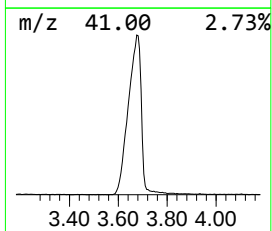
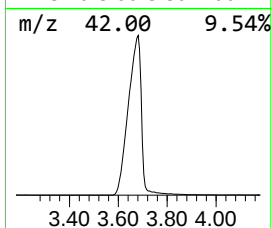
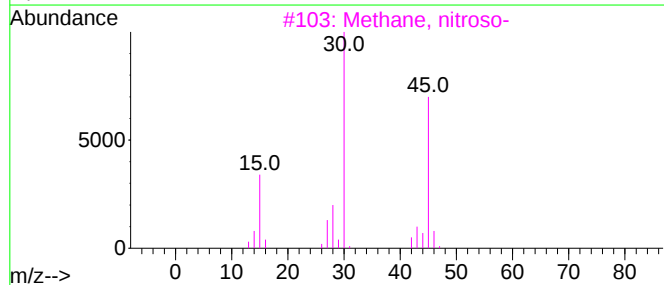
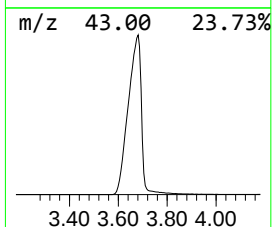
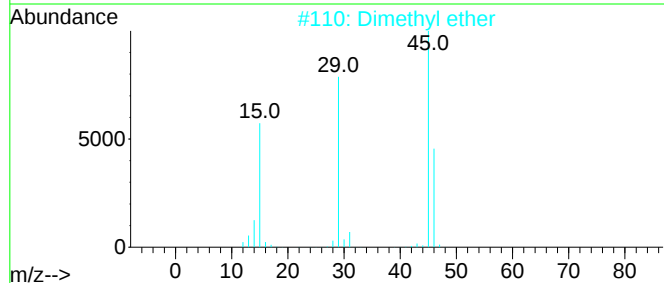
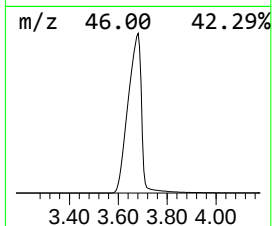
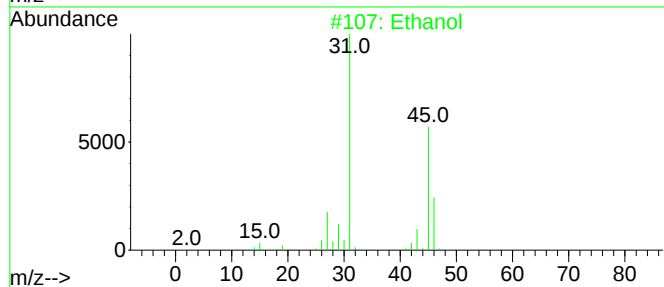
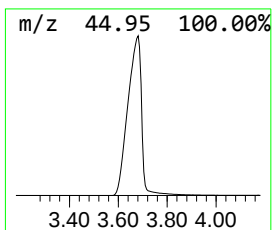
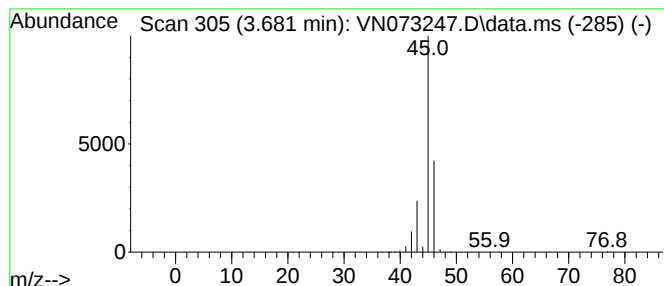
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Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.681	1938.13 ug/l	40218400	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	83
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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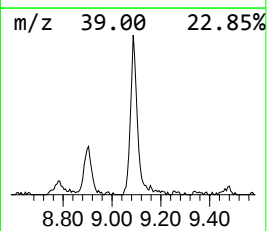
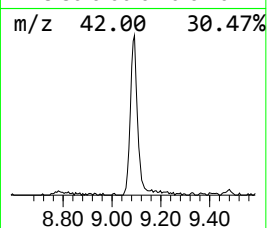
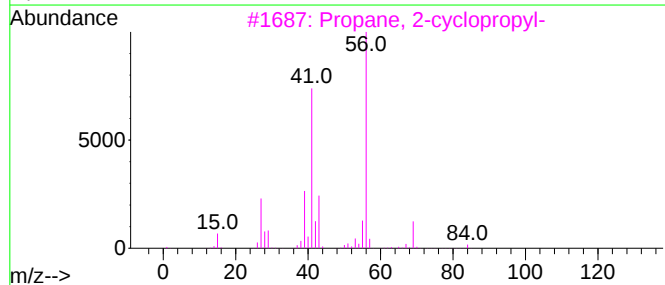
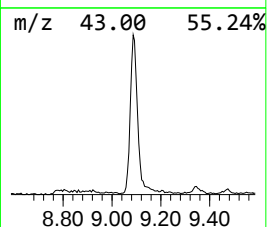
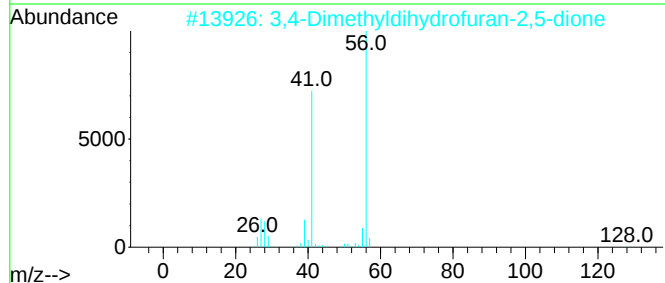
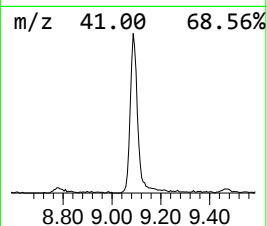
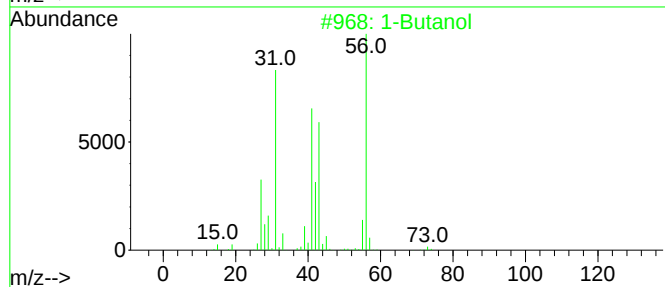
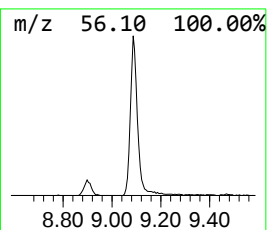
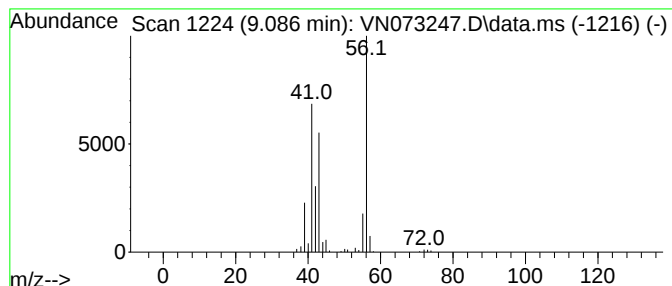
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Peak Number 3 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.086	16.41 ug/l	431631	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	91
2	3,4-Dimethyldihydrofuran-2,5-dione			128	C6H8O3	007475-92-5	40
3	Propane, 2-cyclopropyl-			84	C6H12	003638-35-5	36
4	Butane, 1-chloro-			92	C4H9Cl	000109-69-3	9
5	Oxetane, 2,3,4-trimethyl-, (2.al...			100	C6H12O	032347-12-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.546	585.5	ug/l	12149000	1	8.016	1037560	50.0
Ethanol	3.681	1938.1	ug/l	40218400	1	8.016	1037560	50.0
1-Butanol	9.086	16.4	ug/l	431631	2	8.898	1315500	50.0