

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070124\
Data File : VN082759.D
Acq On : 01 Jul 2024 12:39
Operator : JC\MD
Sample : P3106-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50370

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\82N062724W.M

Title : SW846 8260

Signal : TIC: VN082759.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.930	300	336	338	rBV2	18191390	120360505	100.00%	57.960%
2	7.565	945	954	980	rVB	6629589	15495651	12.87%	7.462%
3	8.606	1123	1131	1149	rVB	6806961	15401685	12.80%	7.417%
4	9.283	1235	1246	1262	rBV	3180458	6262567	5.20%	3.016%
5	10.635	1468	1476	1489	rVB	18554554	32226695	26.78%	15.519%
6	11.077	1543	1551	1561	rBV	762731	1261405	1.05%	0.607%
7	11.965	1694	1702	1711	rVV	1306515	2186600	1.82%	1.053%
8	12.071	1711	1720	1732	rVB	4311291	8131768	6.76%	3.916%
9	12.400	1768	1776	1784	rBV	2605271	4379198	3.64%	2.109%
10	13.482	1953	1960	1977	rVB	1231405	1955840	1.62%	0.942%

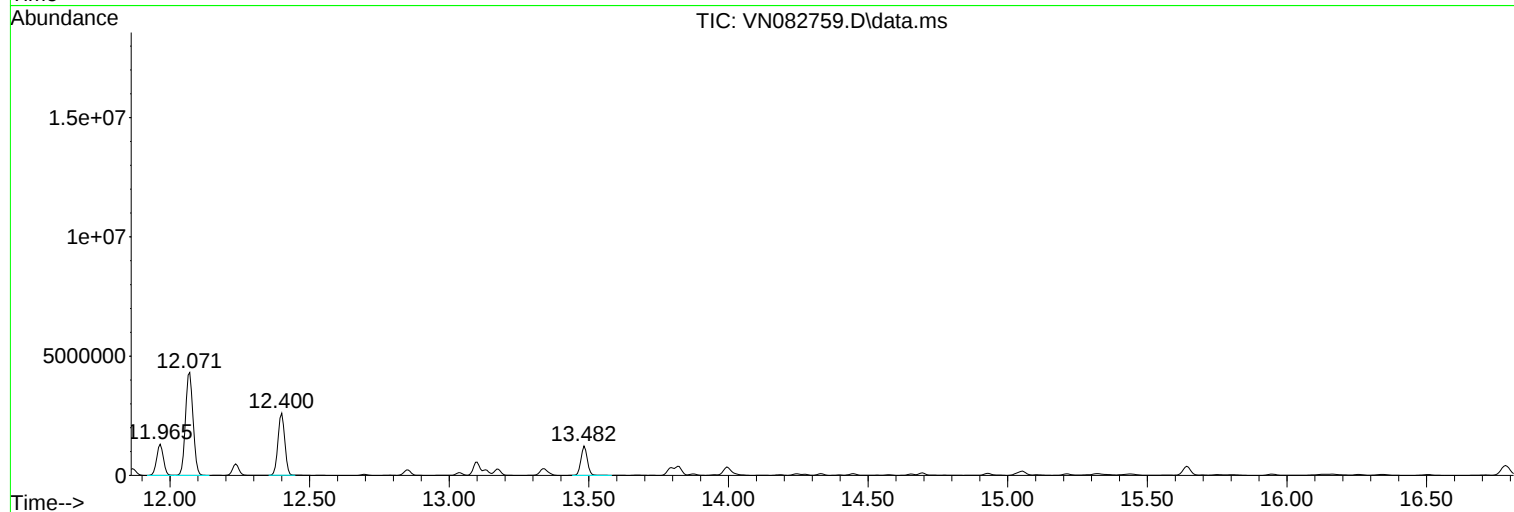
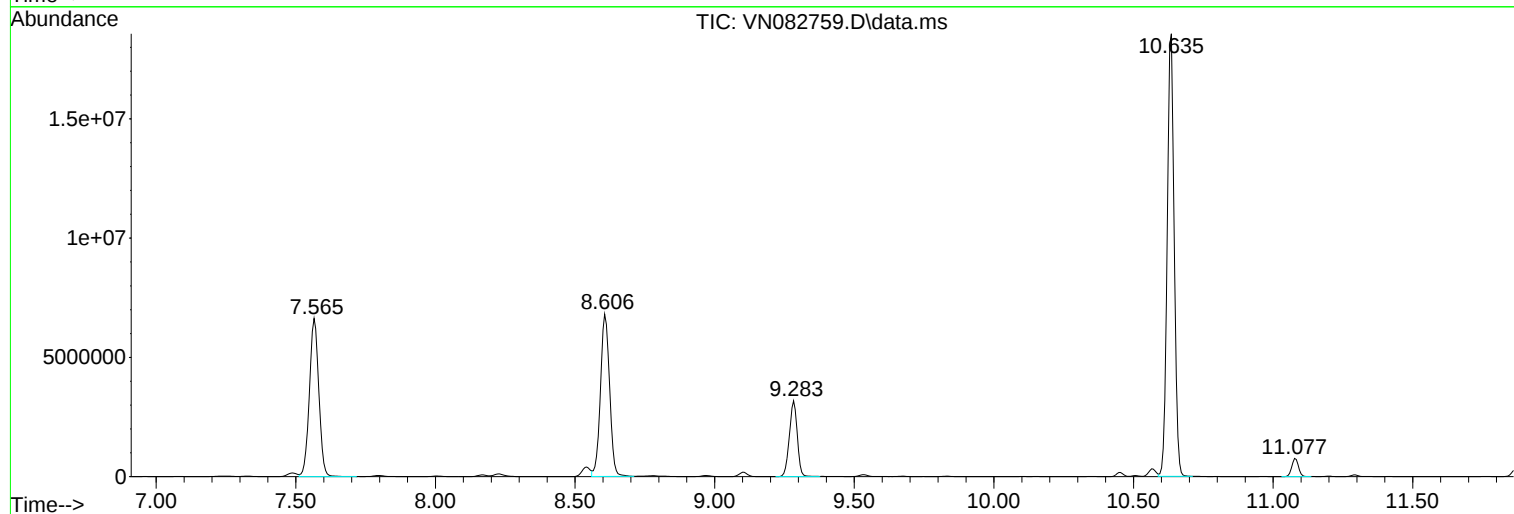
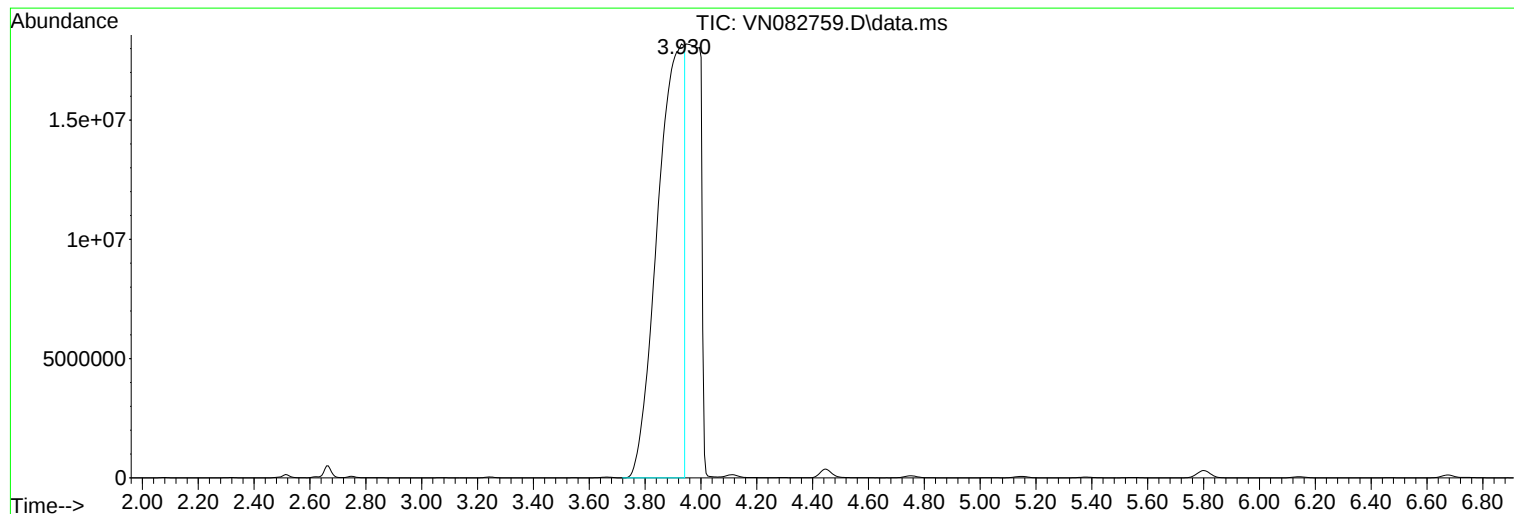
Sum of corrected areas: 207661914

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Quant Title : SW846 8260

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



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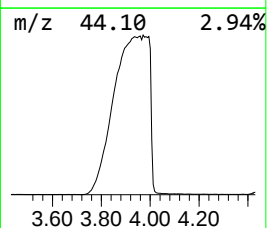
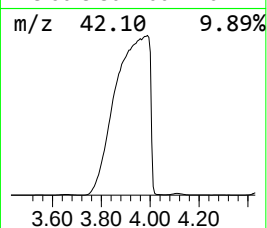
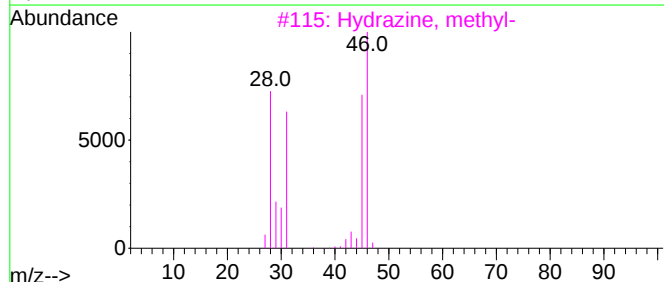
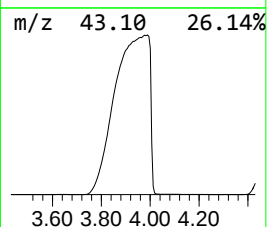
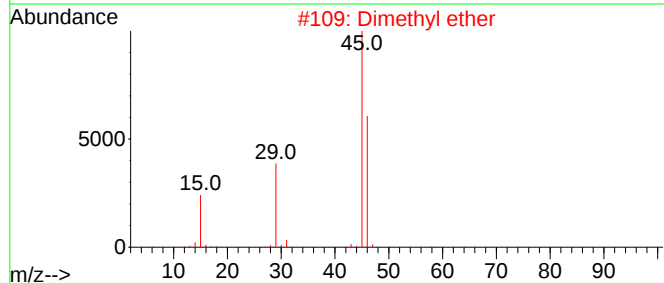
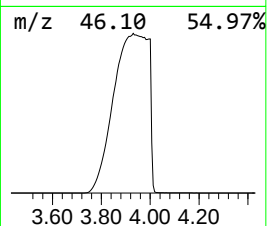
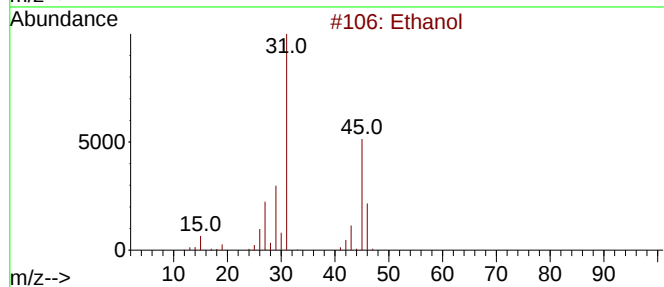
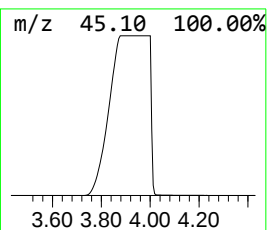
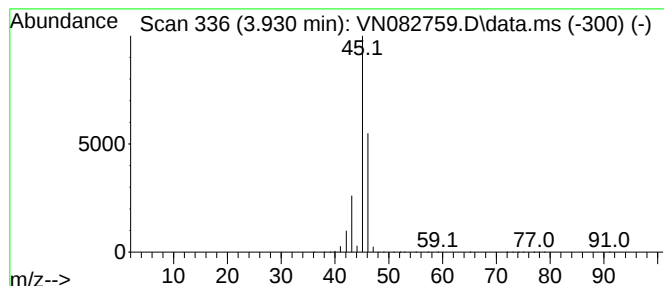
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062724W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.930	390.74 ug/l	120361000	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	86
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Hydrazine, methyl-	46	CH6N2	000060-34-4	9
4			Methane, nitroso-	45	CH3NO	000865-40-7	4
5			Formic acid	46	CH2O2	000064-18-6	4



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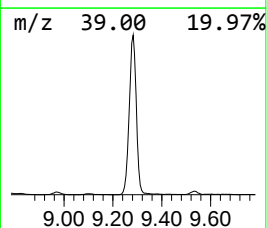
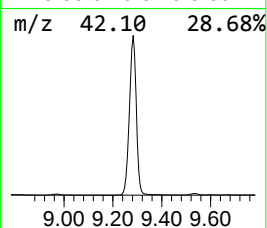
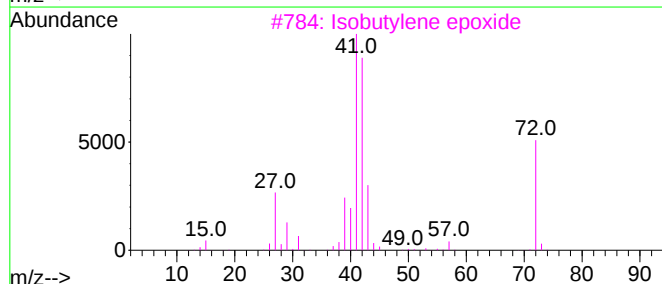
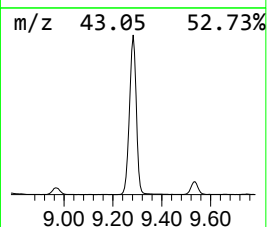
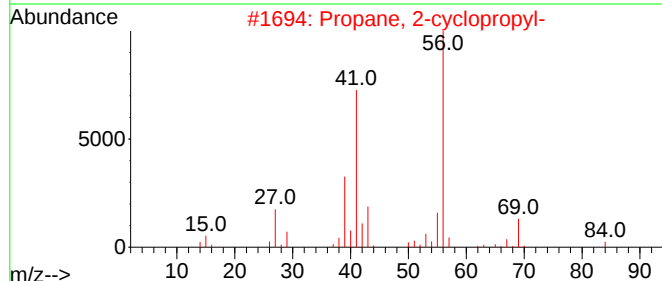
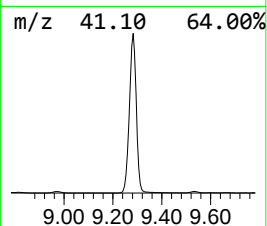
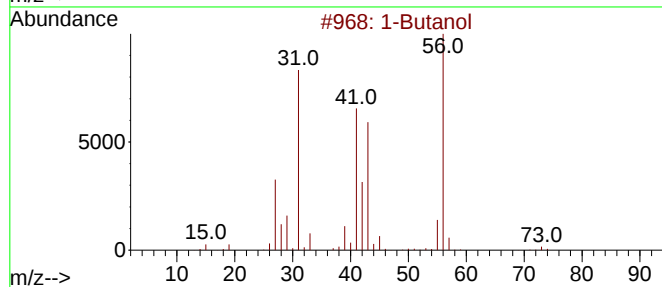
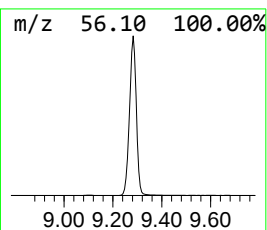
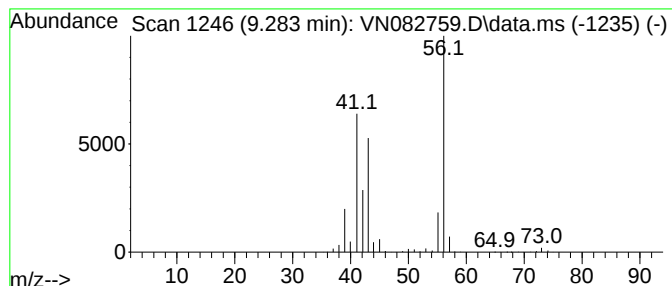
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Peak Number 2 1-Butanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.283	50.00 ug/l	6262570	1,4-Difluorobenzene	9.100	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
3	Isobutylene epoxide	72	C4H8O	000558-30-5	9
4	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9
5	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9



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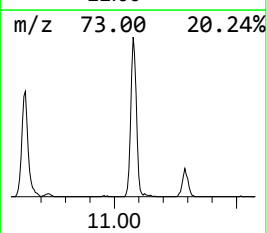
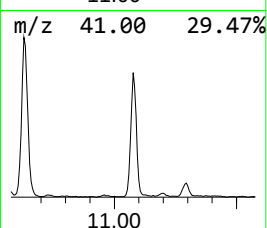
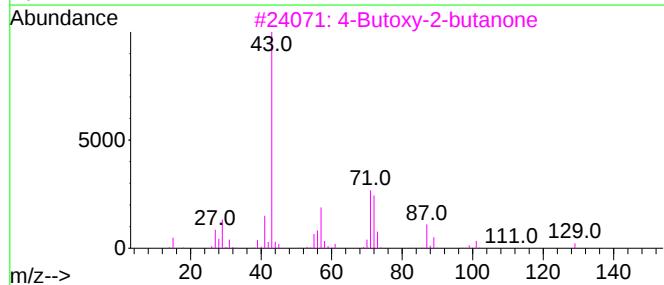
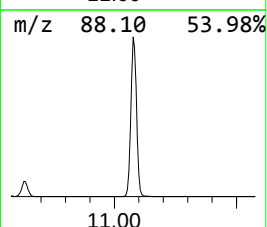
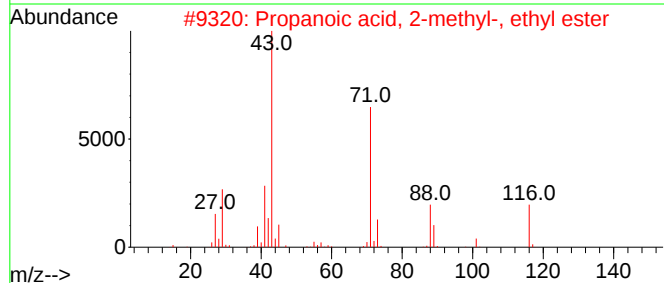
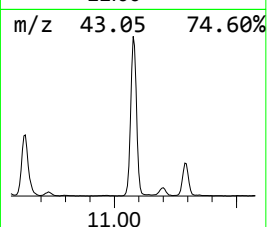
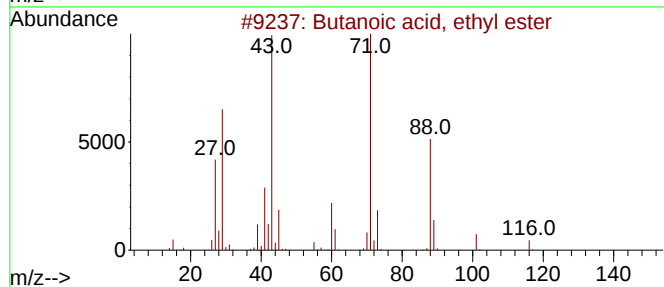
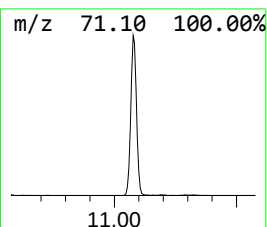
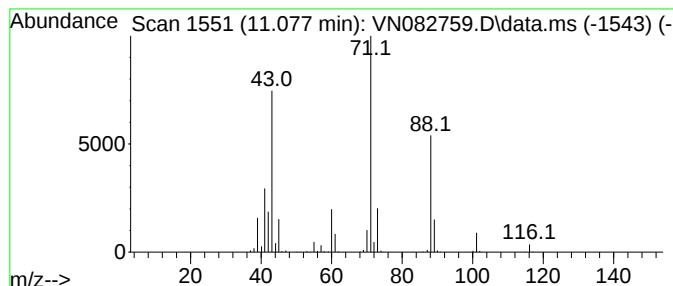
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Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.077	28.84 ug/l	1261410	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42
3			4-Butoxy-2-butanone	144	C8H16O2	030536-44-8	40
4			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	3.930	390.7	ug/l	120361000	1	8.224	15401700	50.0
1-Butanol	9.283	50.0	ug/l	6262570	2	9.100	6262570	50.0
Butanoic acid, ...	11.077	28.8	ug/l	1261410	3	11.865	2186600	50.0