

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100722\
 Data File : VN074818.D
 Acq On : 07 Oct 2022 17:56
 Operator : JC\MD
 Sample : N5009-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 006-4

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\82N100522W.M

Title : SW846 8260

Signal : TIC: VN074818.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.312	38	44	52	rVB	363436	651298	23.86%	5.536%
2	2.418	55	62	63	rBV	52028	84729	3.10%	0.720%
3	2.842	128	134	143	rVB2	167192	548169	20.08%	4.660%
4	8.177	1031	1041	1046	rBV2	369262	878036	32.17%	7.464%
5	8.236	1046	1051	1062	rVB	314750	697750	25.56%	5.931%
6	8.588	1099	1111	1123	rBV3	449973	1034338	37.90%	8.793%
7	9.112	1190	1200	1207	rBV	479722	996931	36.53%	8.475%
8	10.571	1438	1448	1459	rBV	1497680	2729318	100.00%	23.201%
9	11.871	1661	1669	1678	rBV	750114	1361723	49.89%	11.575%
10	12.853	1826	1836	1848	rBV	824001	1417569	51.94%	12.050%
11	13.794	1985	1996	2008	rBV	798858	1364003	49.98%	11.595%

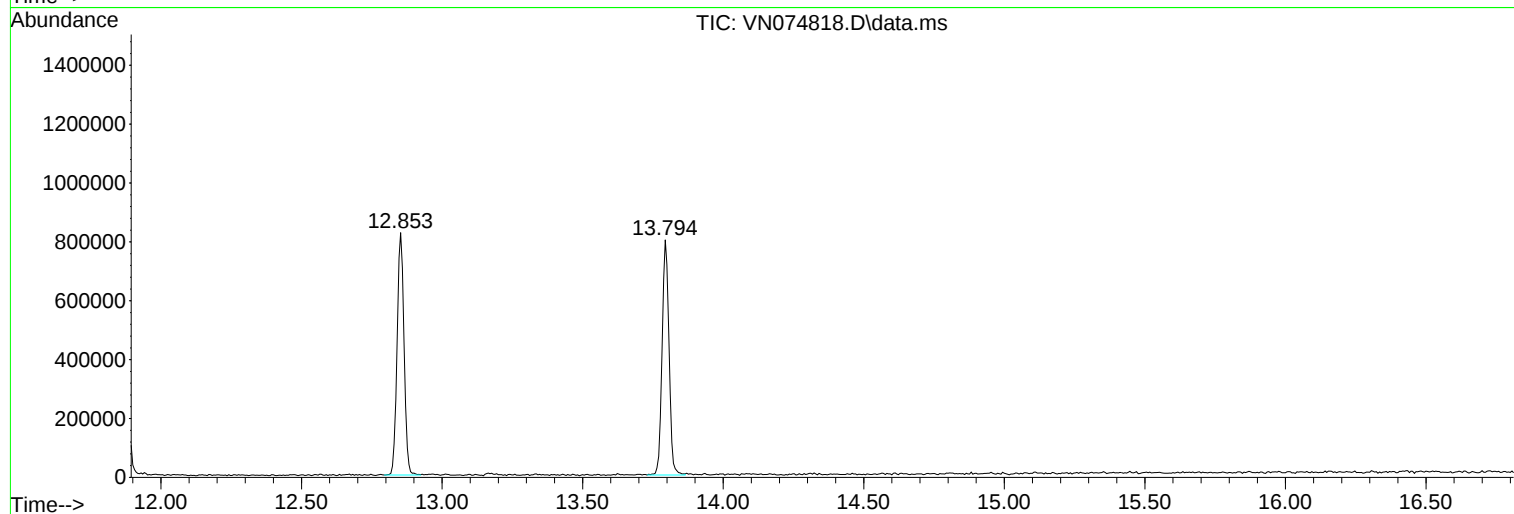
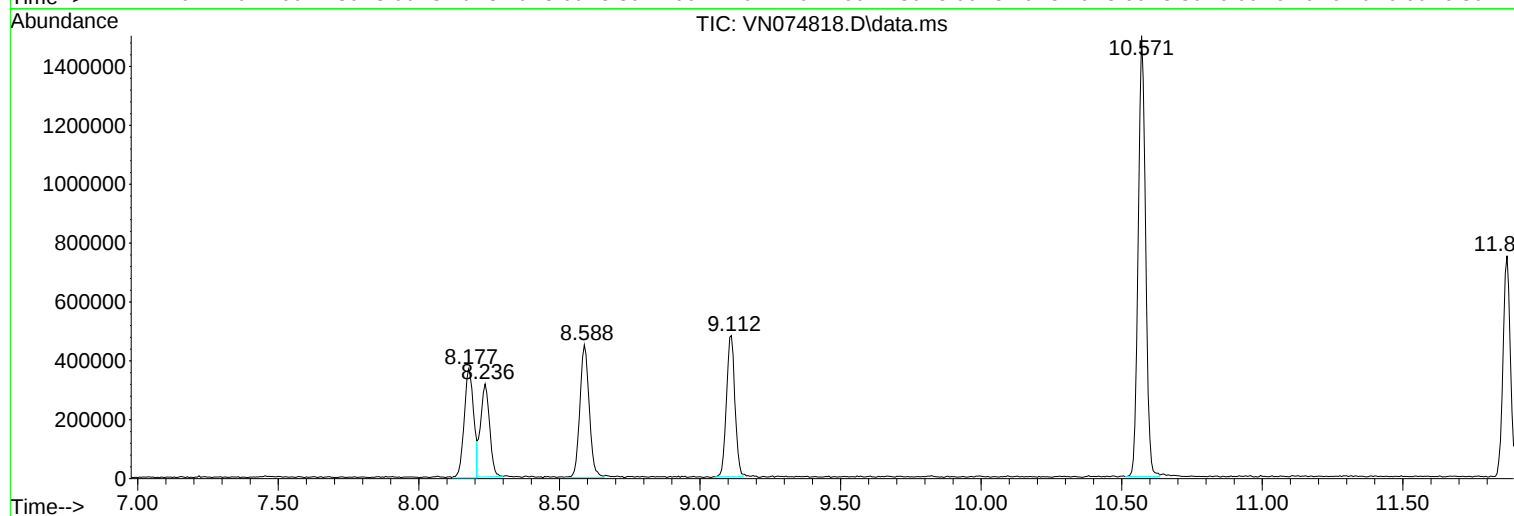
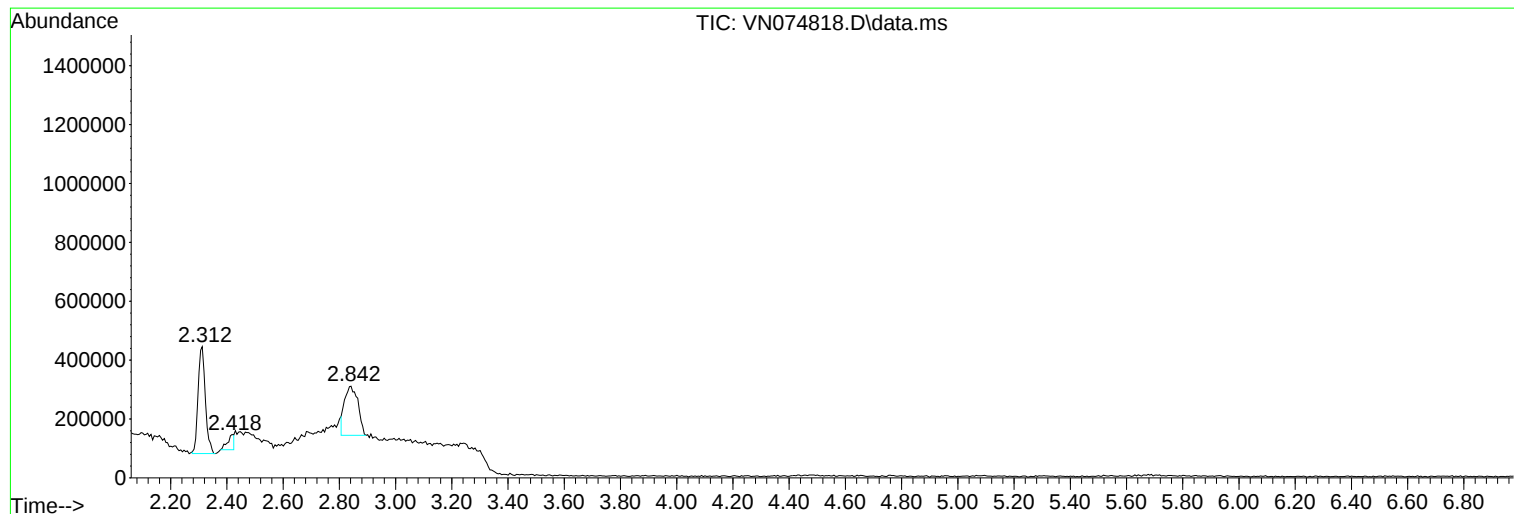
Sum of corrected areas: 11763864

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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



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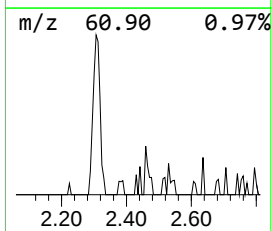
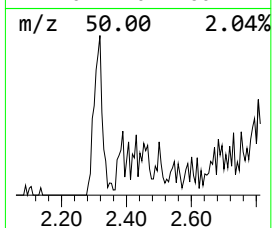
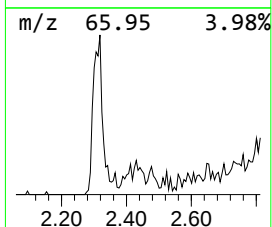
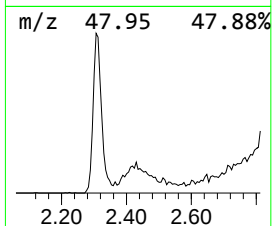
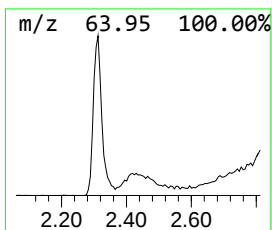
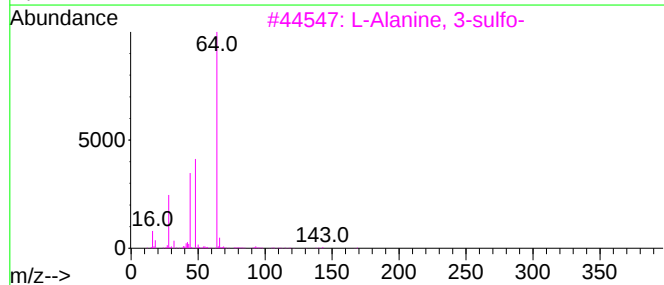
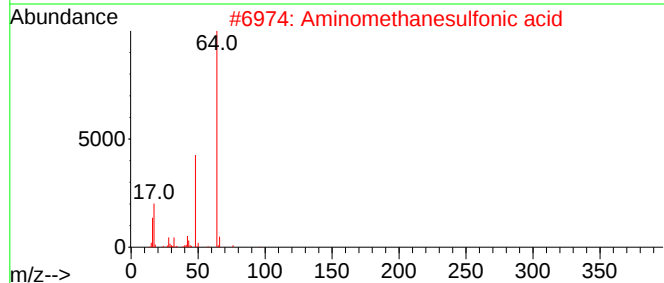
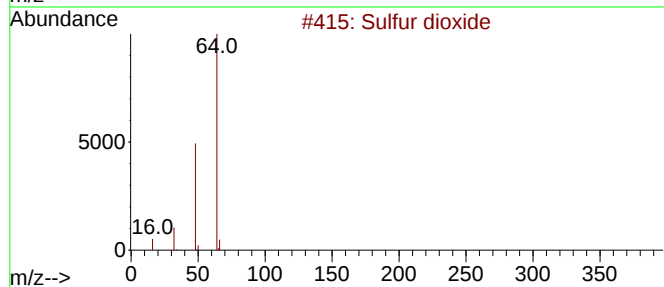
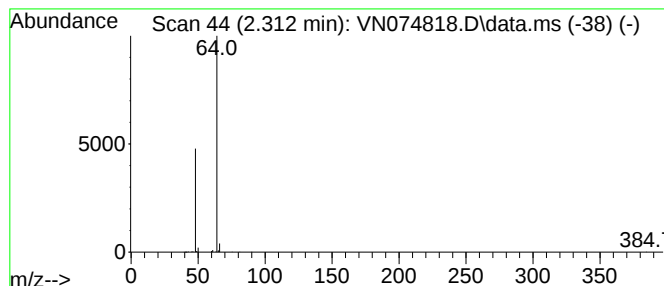
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.312	46.67 ug/l	651298	Pentafluorobenzene	8.236

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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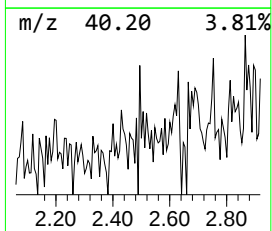
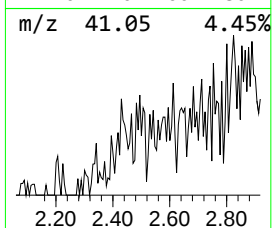
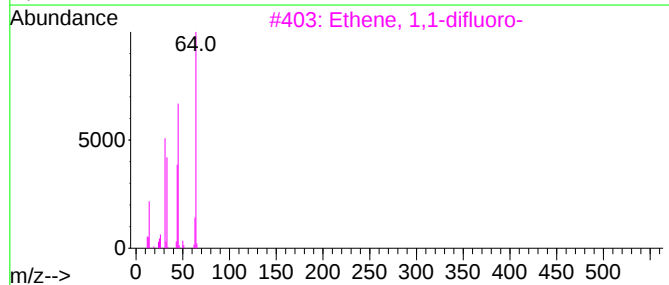
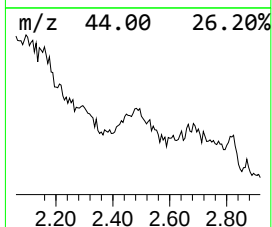
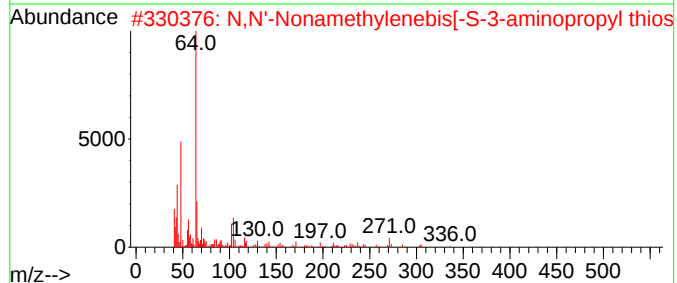
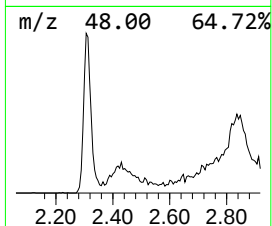
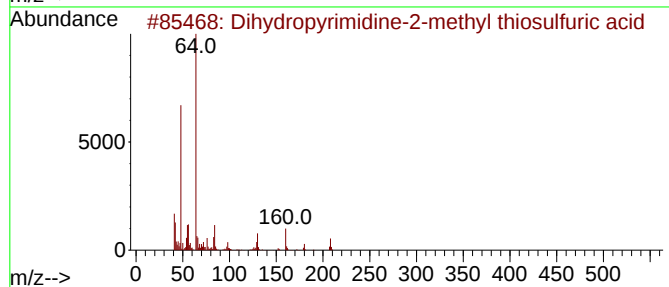
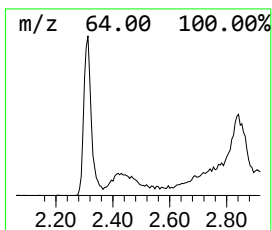
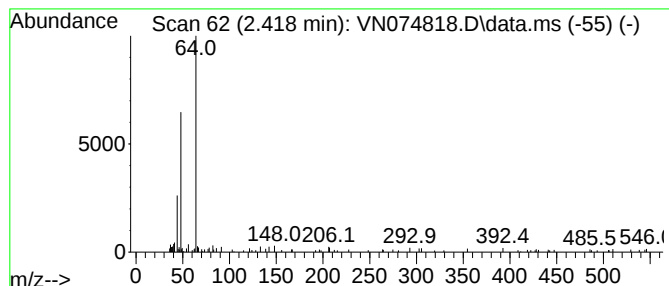
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Peak Number 2 Dihydropyrimidine-2-methyl ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.418	6.07 ug/l	84729	Pentafluorobenzene	8.236

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	64
2			N,N'-Nonamethylenebis[-S-3-amino...	466	C15H34N2O6S4	035871-58-0	64
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	9
4			Sulfur dioxide	64	O2S	007446-09-5	9
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	9



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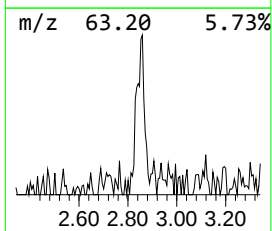
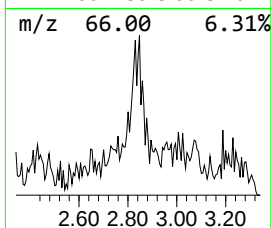
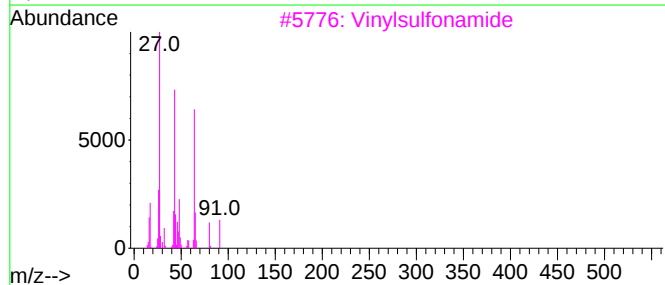
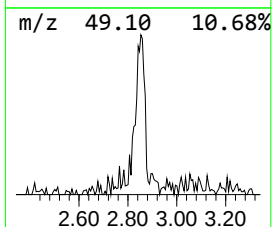
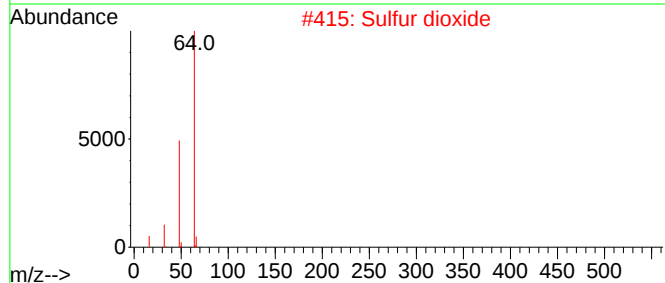
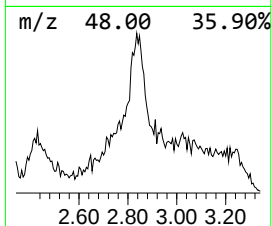
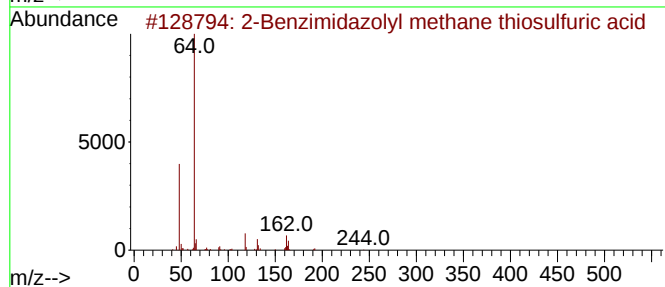
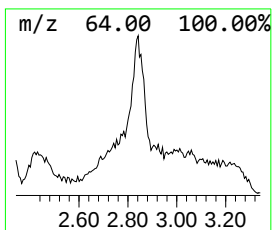
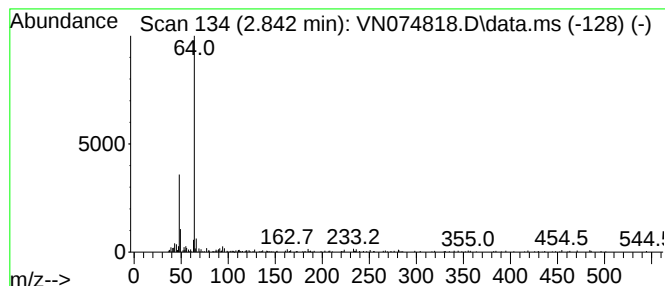
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Peak Number 3 2-Benzimidazolyl methane th... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.	
2.842	39.28 ug/l	548169	Pentafluorobenzene			8.236	
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	78
2			Sulfur dioxide	64	O2S	007446-09-5	64
3			Vinylsulfonamide	107	C2H5NO2S	002386-58-5	64
4			N,N'-Nonamethylenebis[-S-3-amino...	466	C15H34N2O6S4	035871-58-0	43
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.312	46.7	ug/l	651298	1	8.236	697750	50.0
Dihydropyrimidi...	2.418	6.1	ug/l	84729	1	8.236	697750	50.0
2-Benzimidazoly...	2.842	39.3	ug/l	548169	1	8.236	697750	50.0