

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100722\
 Data File : VN074813.D
 Acq On : 07 Oct 2022 15:55
 Operator : JC\MD
 Sample : N4979-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 251032-4

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: VN074813.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	51	rBV	305844	545053	18.26%	4.153%
2	2.412	54	61	62	rBV4	49943	98572	3.30%	0.751%
3	2.636	96	99	100	rBV2	26025	31605	1.06%	0.241%
4	2.853	130	136	143	rVB3	166953	479241	16.05%	3.651%
5	8.177	1030	1041	1046	rBV2	383805	945582	31.67%	7.204%
6	8.235	1046	1051	1059	rVB	390785	863474	28.92%	6.578%
7	8.588	1102	1111	1125	rBV2	470904	1086588	36.39%	8.278%
8	9.106	1190	1199	1209	rBV2	578511	1215548	40.71%	9.261%
9	10.571	1439	1448	1457	rBV	1593339	2985551	100.00%	22.746%
10	11.871	1660	1669	1680	rBV	899642	1639509	54.91%	12.491%
11	12.853	1827	1836	1848	rVB	896202	1564425	52.40%	11.919%
12	13.794	1988	1996	2004	rBV2	959283	1670683	55.96%	12.728%

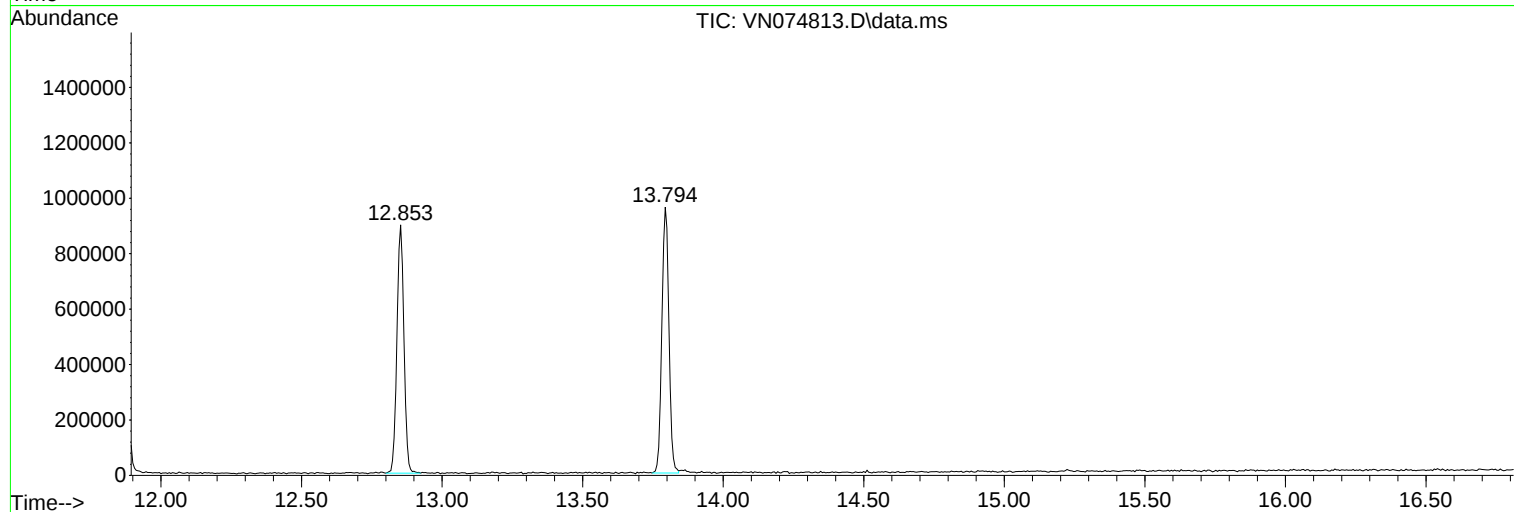
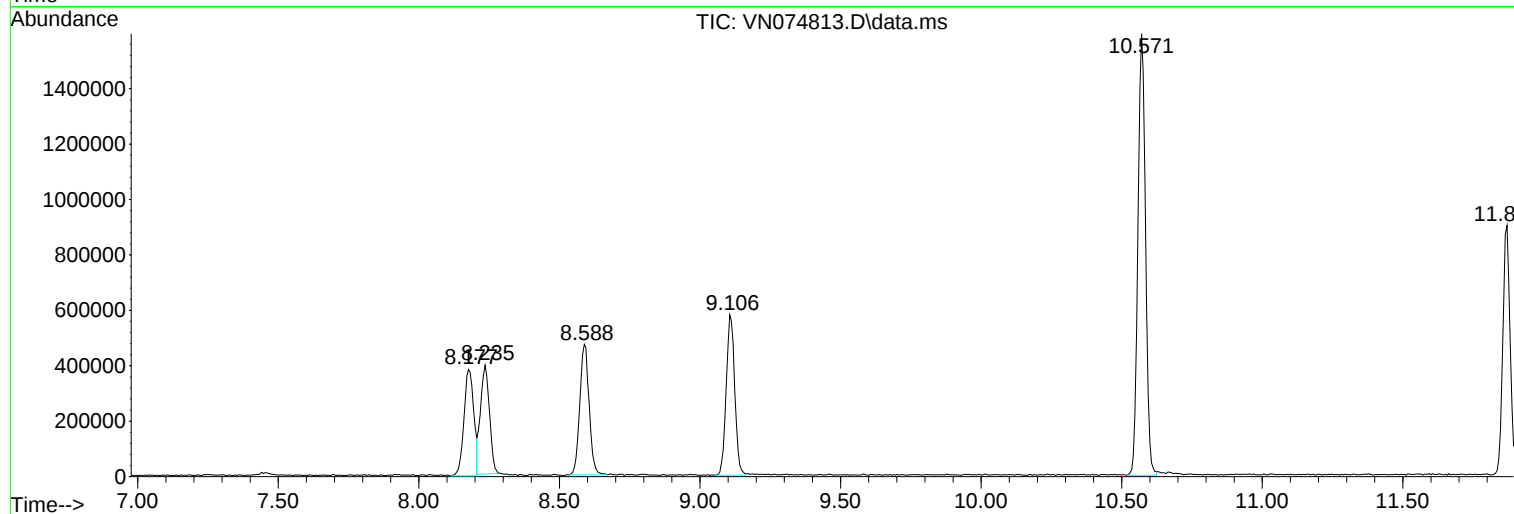
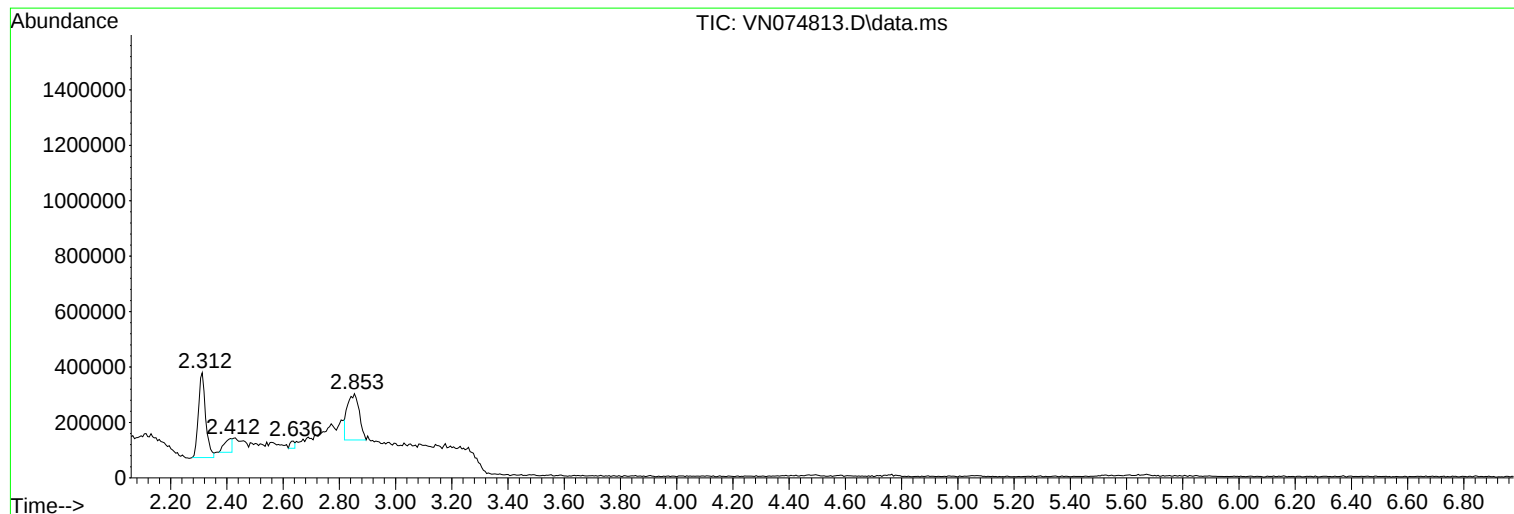
Sum of corrected areas: 13125831

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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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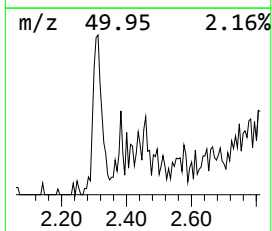
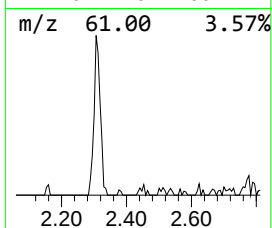
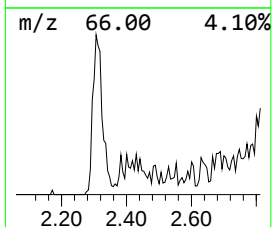
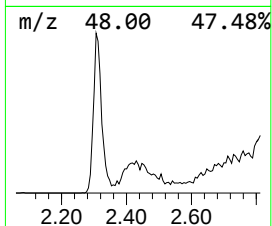
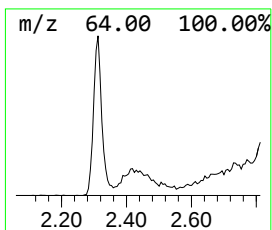
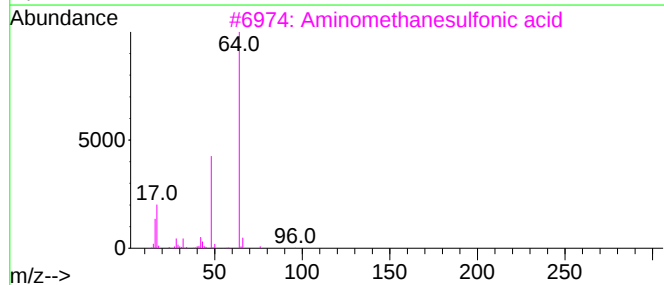
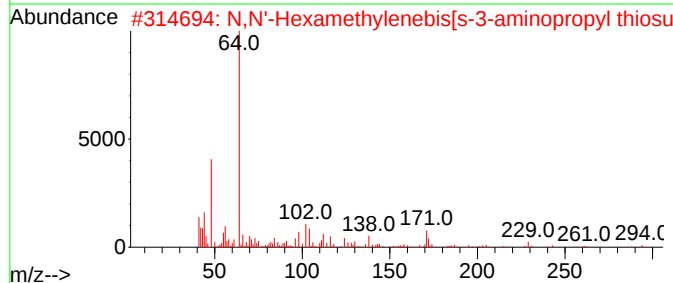
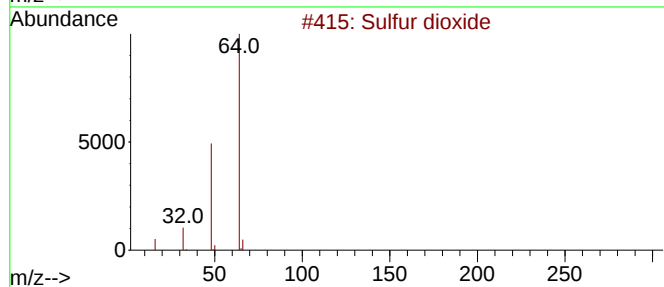
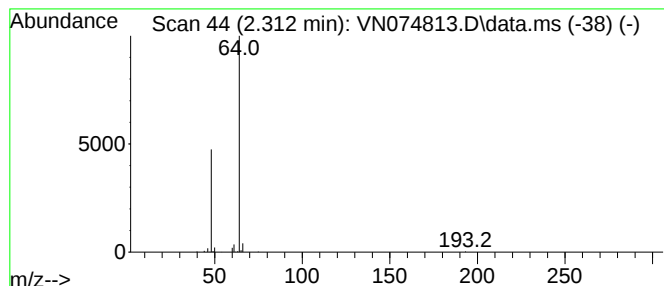
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.312	31.56 ug/l	545053	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			1,1,1,2,2,3,3,4,4,5,5-Undecaflu...	602	C10F22O2S	1000486-78-5	64
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	64



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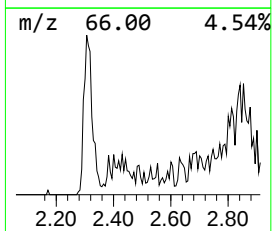
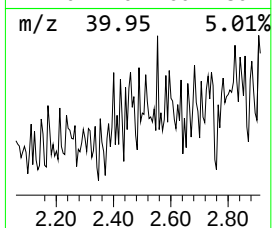
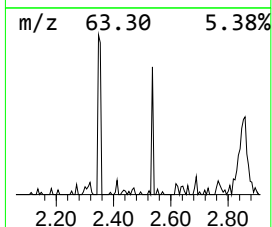
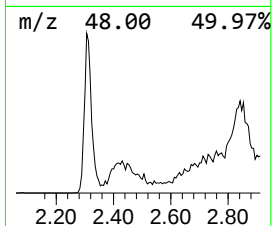
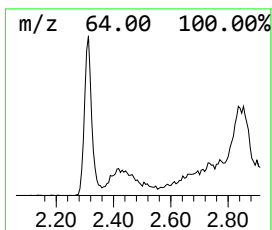
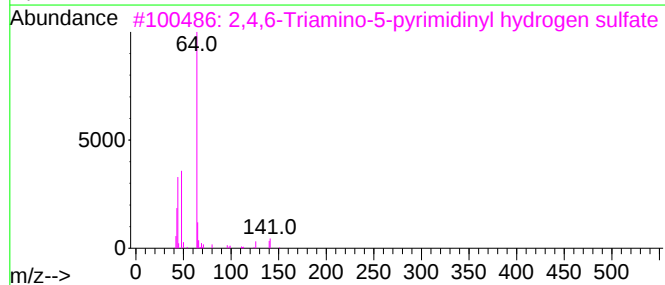
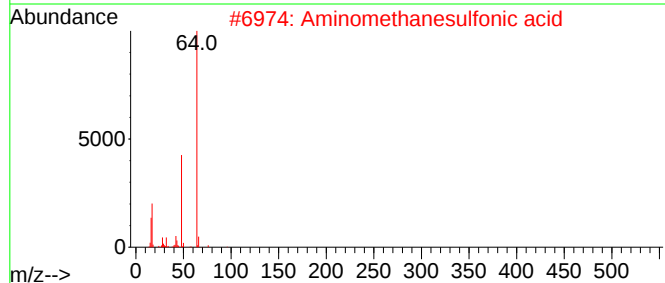
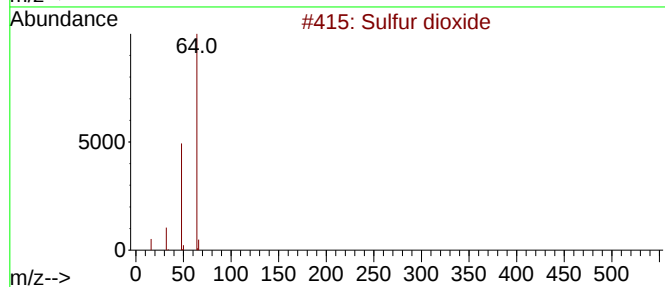
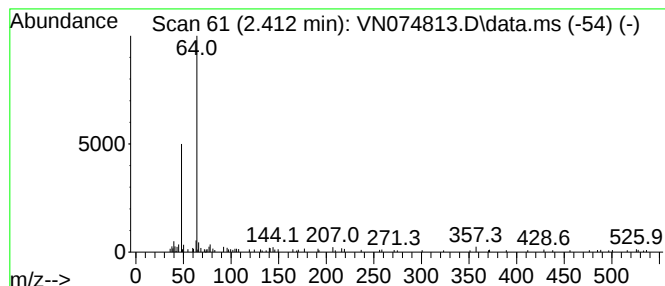
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Aminomethanesulfonic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.412	5.71 ug/l	98572	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	74
4			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	74
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	74



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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.312	31.6	ug/l	545053	1	8.235	863474	50.0
Aminomethanesul...	2.412	5.7	ug/l	98572	1	8.235	863474	50.0