

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041222\
 Data File : VX028069.D
 Acq On : 12 Apr 2022 20:16
 Operator : JC/MD
 Sample : N2333-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-14R

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_X\Method\82X041222W.M

Title : SW846 8260

Signal : TIC: VX028069.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.288	26	33	43	rBV2	32753	126023	9.81%	1.766%
2	1.569	73	79	94	rVB4	41158	137420	10.69%	1.926%
3	2.782	269	278	285	rVB3	10339	23889	1.86%	0.335%
4	5.391	694	706	720	rBV	152061	455885	35.48%	6.388%
5	5.556	722	733	750	rVB	242302	680876	52.98%	9.541%
6	5.958	788	799	813	rBV	162815	435038	33.85%	6.096%
7	6.763	920	931	946	rBV	386406	924633	71.95%	12.956%
8	8.653	1234	1241	1250	rBV	808668	1285036	100.00%	18.006%
9	10.055	1465	1471	1483	rBV	872641	1145342	89.13%	16.049%
10	11.079	1634	1639	1651	rBV	662218	855901	66.61%	11.993%
11	12.024	1789	1794	1801	rBV	866852	1066496	82.99%	14.944%

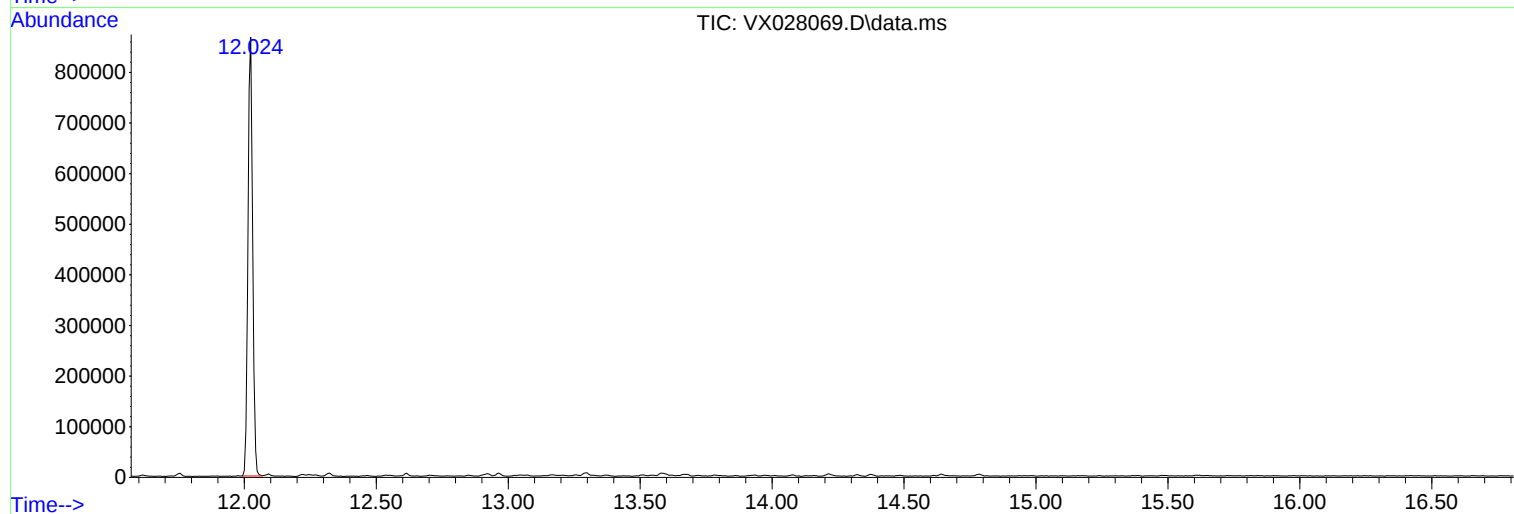
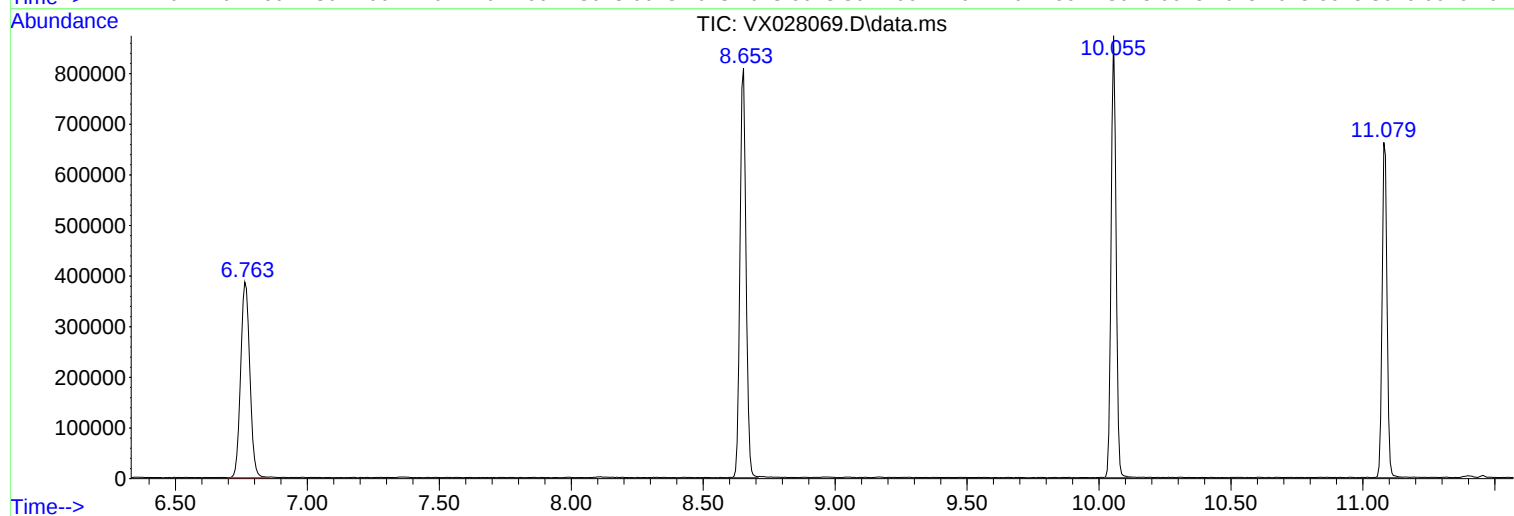
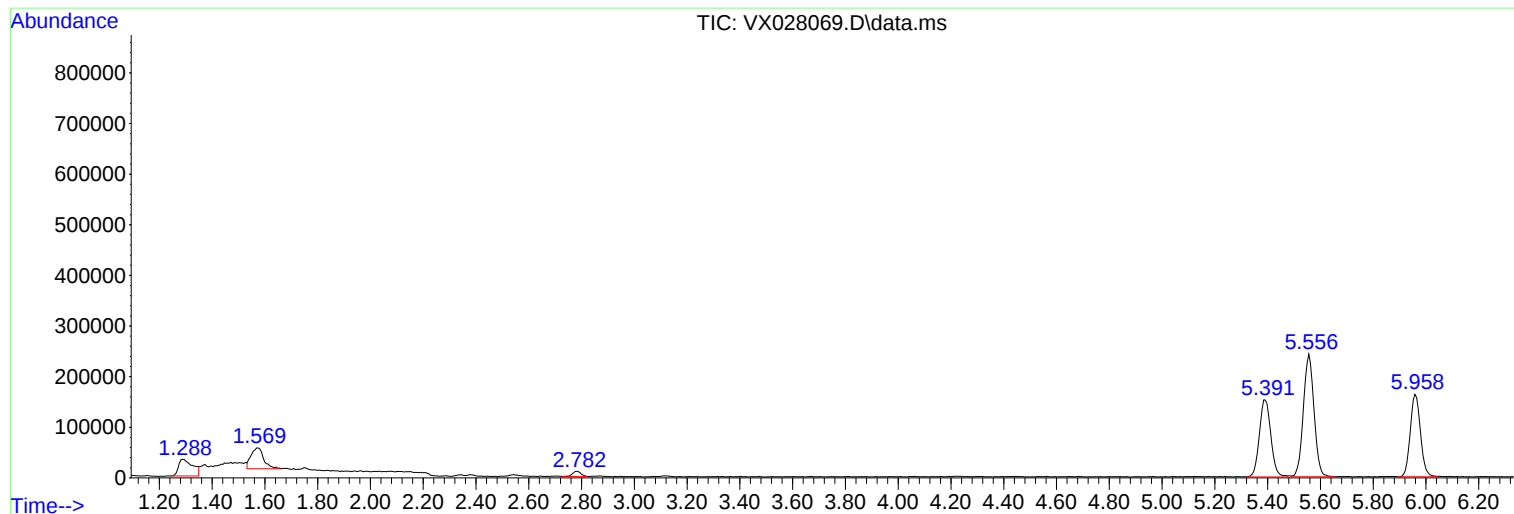
Sum of corrected areas: 7136539

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
Quant Title : SW846 8260

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



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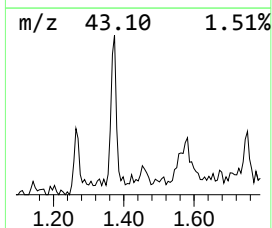
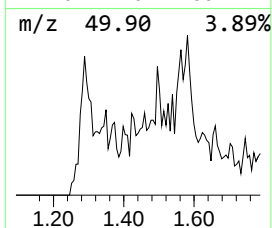
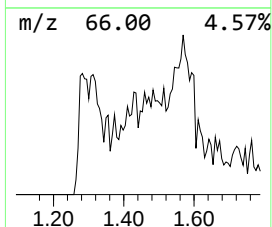
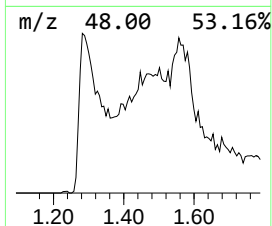
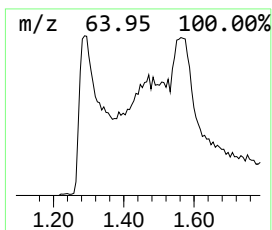
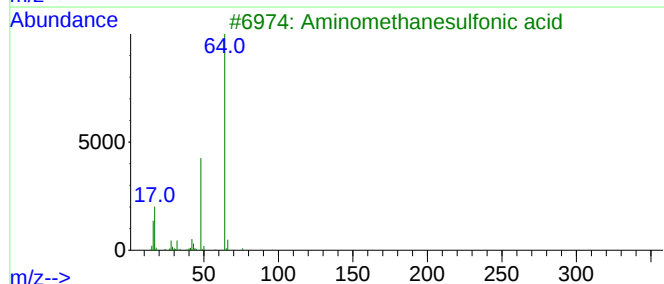
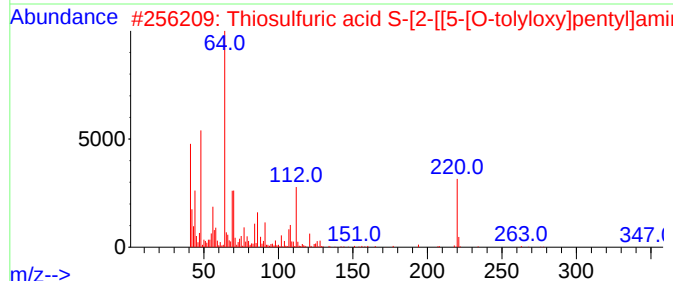
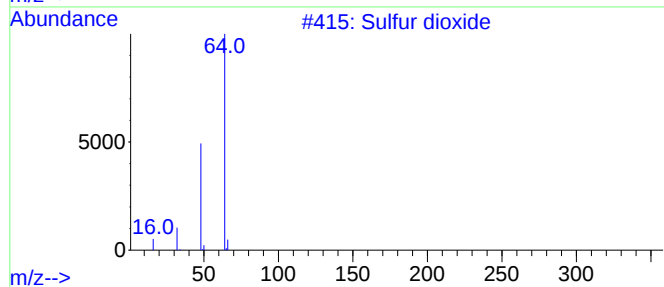
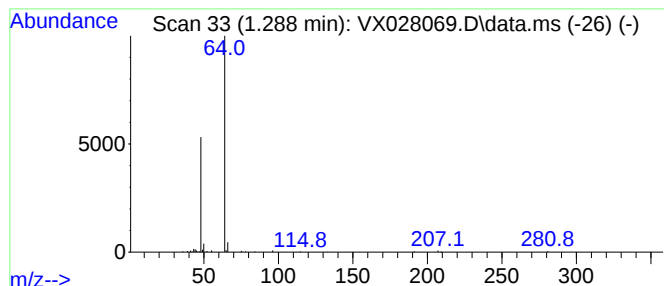
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.288	9.25 ug/l	126023	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Thiosulfuric acid S-[2-[[5-[0-to...	347	C15H25NO4S2	038920-47-7	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	9
5			2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	9



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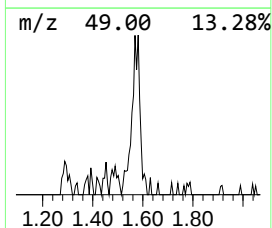
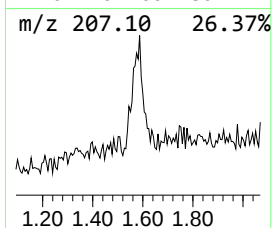
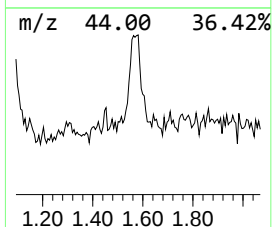
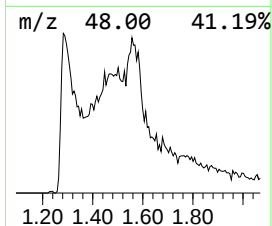
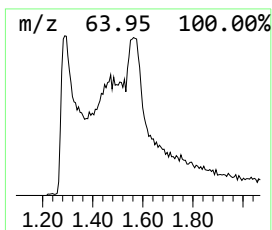
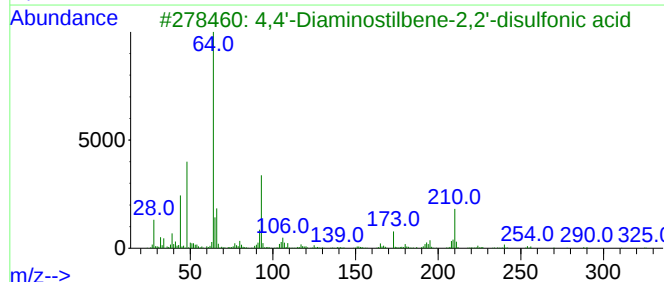
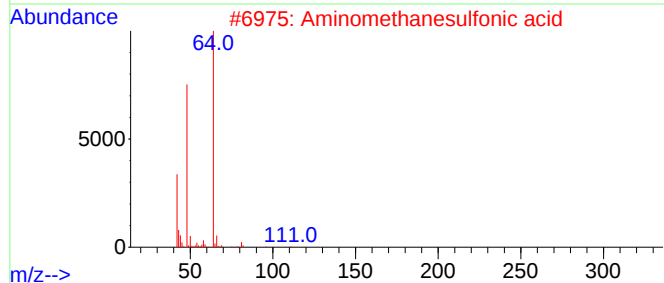
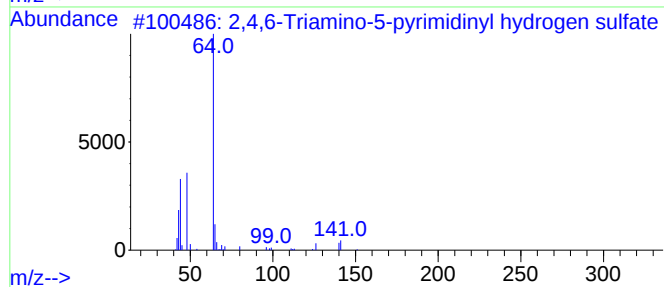
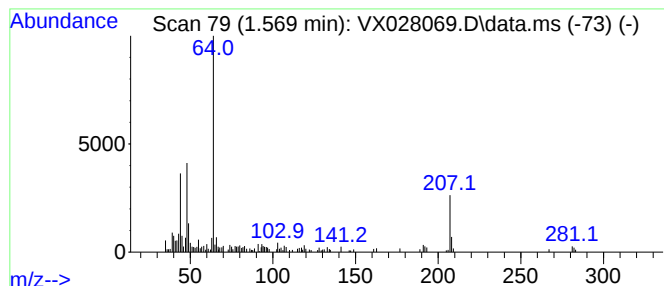
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Peak Number 2 2,4,6-Triamino-5-pyrimidiny... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.569	10.09 ug/l	137420	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	78
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	72
3			4,4'-Diaminostilbene-2,2'-disulf...	370	C14H14N2O6S2	000081-11-8	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	56
5			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.288	9.3	ug/l	126023	1	5.556	680876	50.0
2,4,6-Triamino-...	1.569	10.1	ug/l	137420	1	5.556	680876	50.0