

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122623\
Data File : VX039460.D
Acq On : 26 Dec 2023 12:26
Operator : JC/MD
Sample : VX1226MBL01
Misc : 5.00g/10mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VX1226MBL01

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\82X121323W.M

Title : SW846 8260

Signal : TIC: VX039460.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	37	rBV	17685	35632	4.97%	0.938%
2	1.557	70	77	82	rBV5	4442	9594	1.34%	0.252%
3	5.385	694	705	721	rBV3	75581	222358	30.99%	5.851%
4	5.550	721	732	749	rVB	112786	323684	45.11%	8.518%
5	5.952	788	798	813	rBV	88477	232039	32.34%	6.106%
6	6.757	921	930	945	rBV	209049	500997	69.82%	13.184%
7	8.647	1233	1240	1254	rBV	454538	717510	100.00%	18.881%
8	10.049	1465	1470	1491	rVB	462310	672001	93.66%	17.684%
9	11.079	1634	1639	1650	rBV	387695	496172	69.15%	13.057%
10	12.024	1788	1794	1810	rBV	437260	590105	82.24%	15.529%

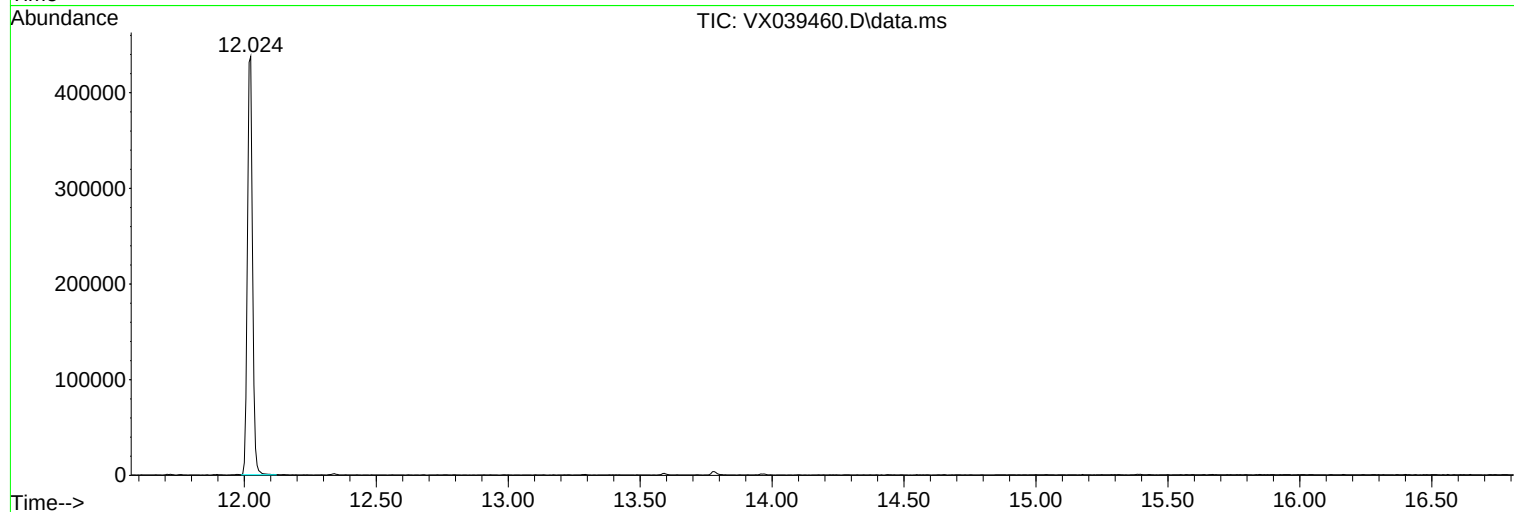
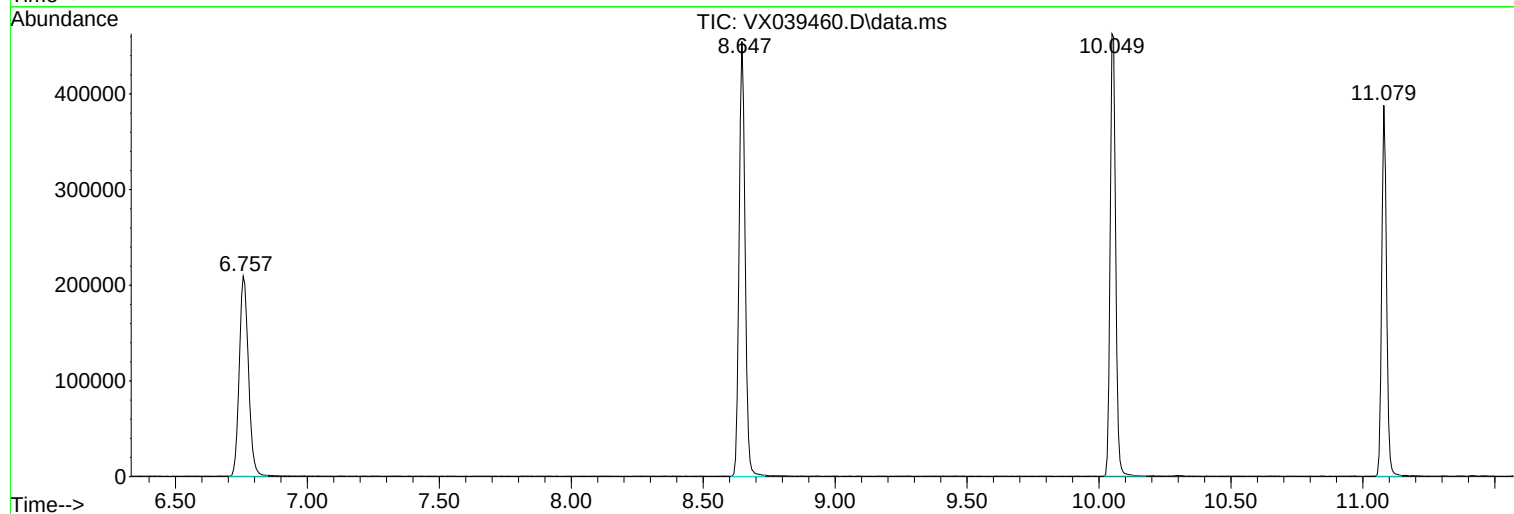
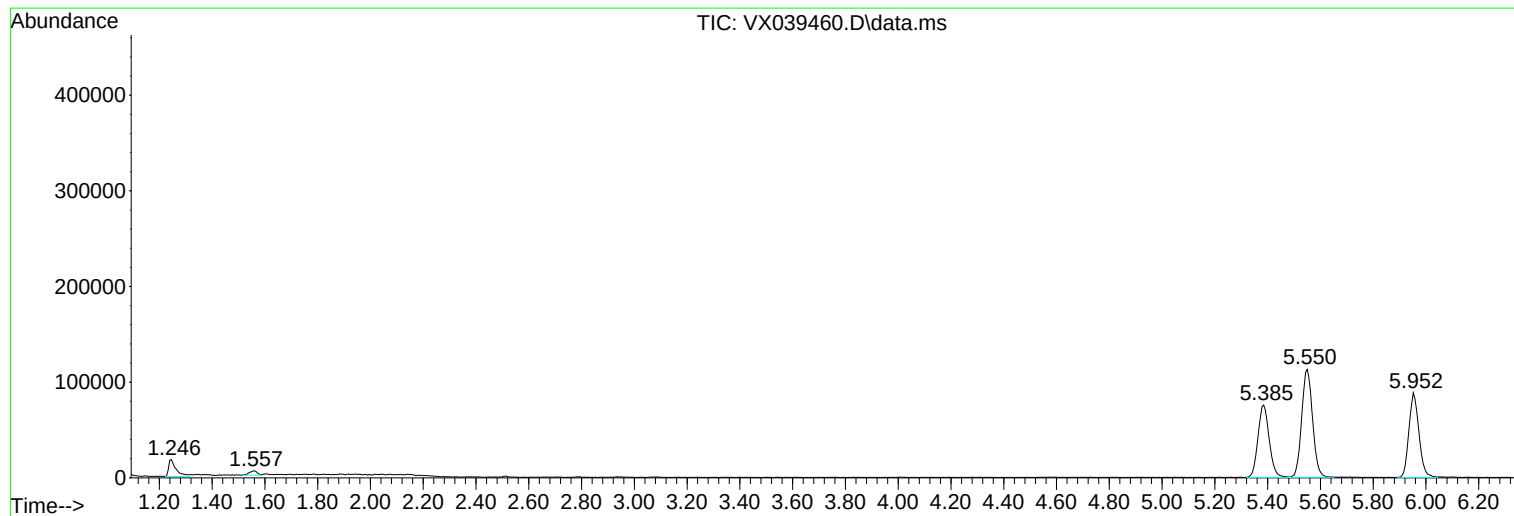
Sum of corrected areas: 3800092

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



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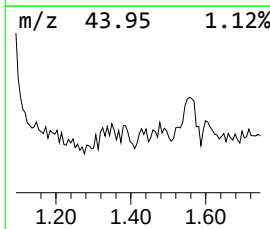
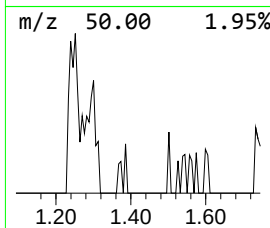
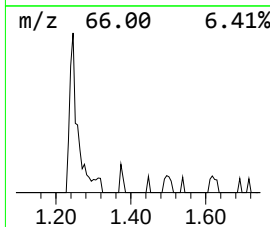
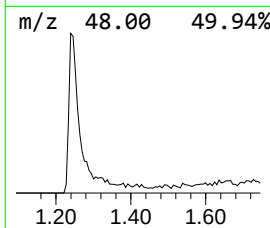
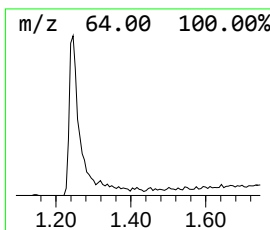
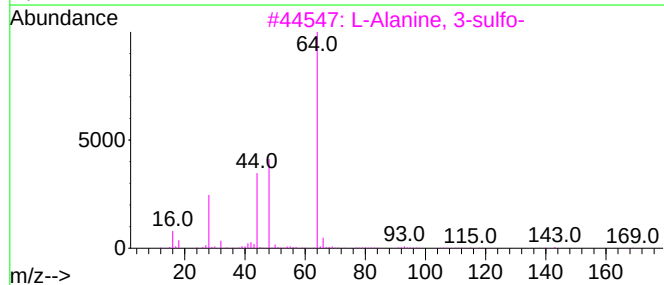
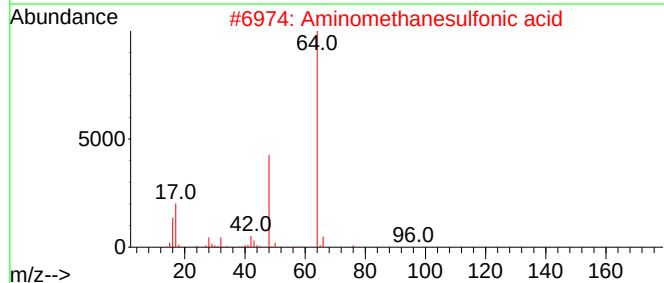
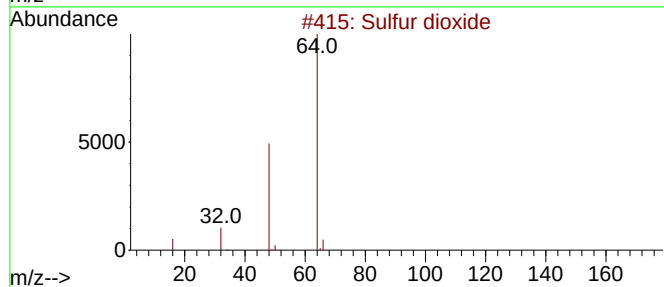
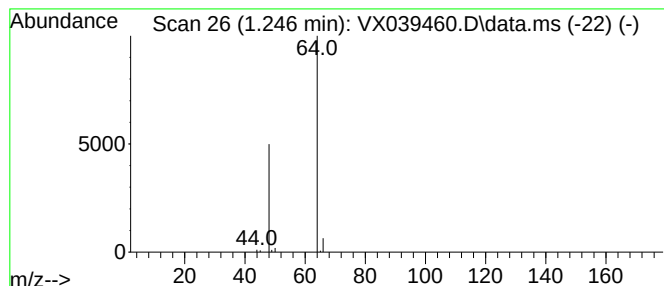
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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.
1.246	5.50 ug/l	35632	Pentafluorobenzene	5.550

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	9
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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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.246	5.5	ug/l	35632	1	5.550	323684	50.0