

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022023\
Data File : VX034180.D
Acq On : 20 Feb 2023 12:17
Operator : JC/MD
Sample : 01593-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TB-2023-2-16

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M

Title : SW846 8260

Signal : TIC: VX034180.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	24	29	44	rBV	31721	112306	5.65%	1.098%
2	5.385	692	705	721	rBV	220406	654752	32.97%	6.400%
3	5.550	721	732	753	rVB	365438	1060831	53.41%	10.369%
4	5.958	787	799	816	rBV	240030	649072	32.68%	6.344%
5	6.763	921	931	951	rBV	588362	1423799	71.69%	13.917%
6	8.647	1233	1240	1254	rBV	1265825	1986106	100.00%	19.413%
7	10.055	1465	1471	1483	rBV	1190412	1651136	83.13%	16.139%
8	11.079	1634	1639	1652	rBV	937620	1219860	61.42%	11.923%
9	12.024	1788	1794	1808	rBV	1127043	1472995	74.16%	14.398%

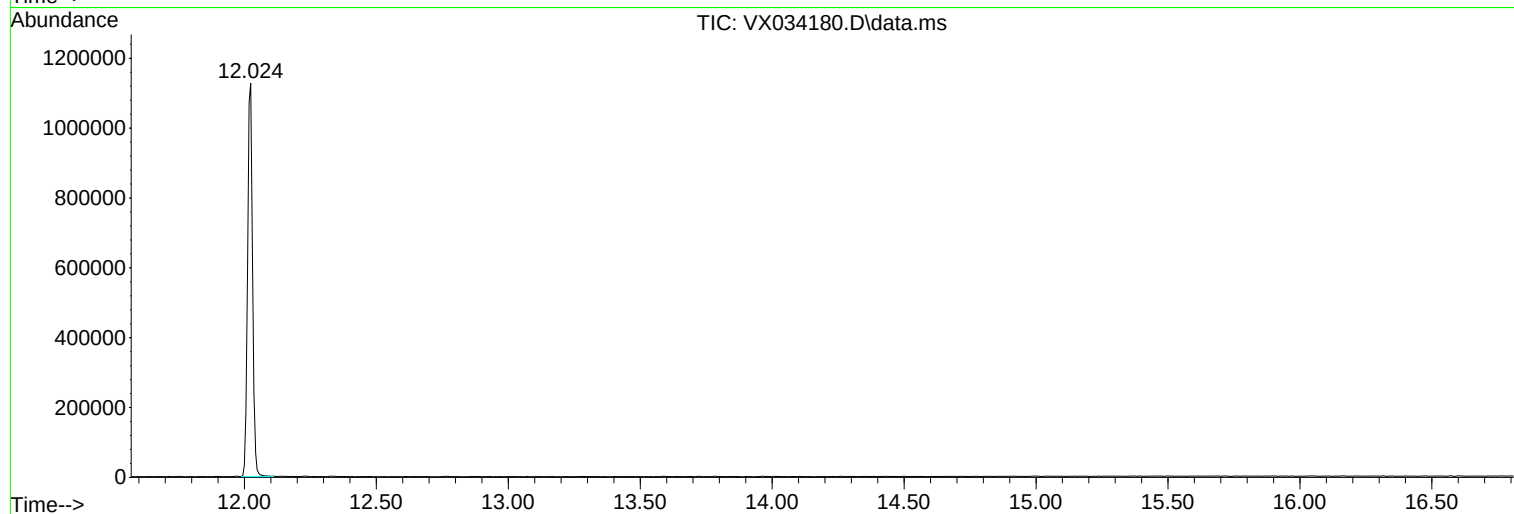
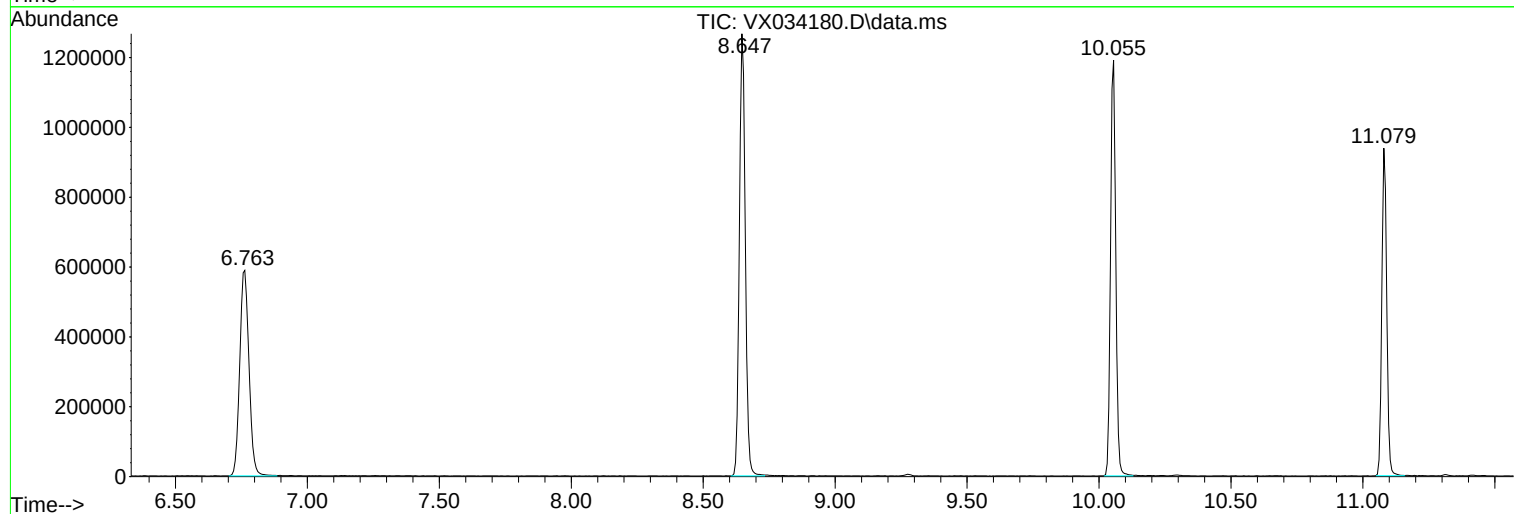
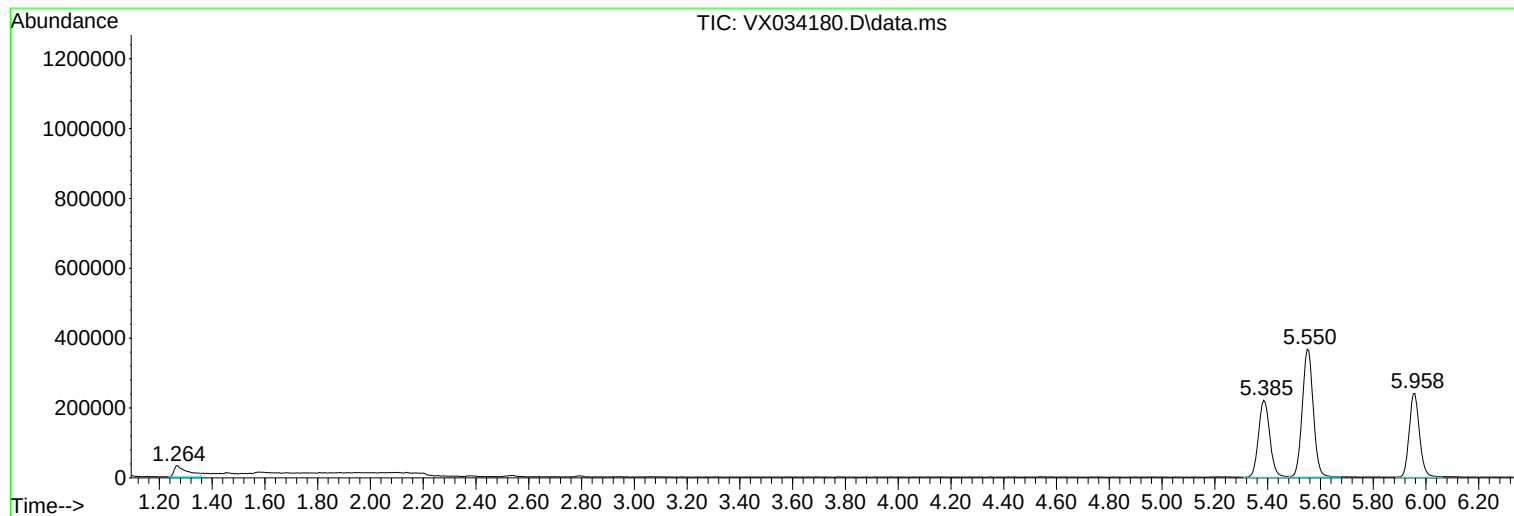
Sum of corrected areas: 10230857

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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



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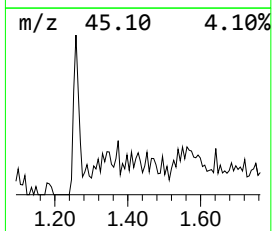
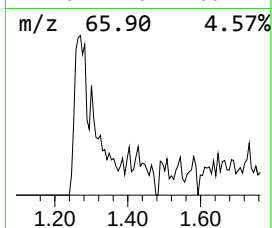
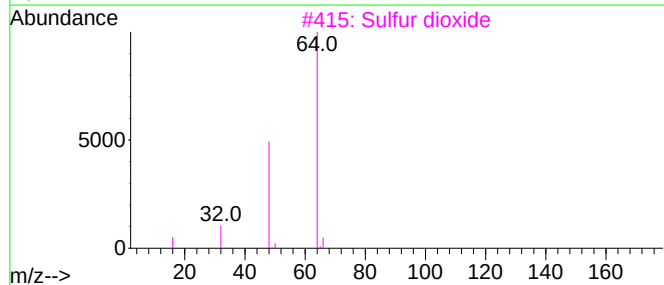
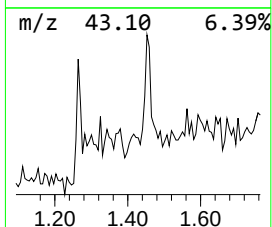
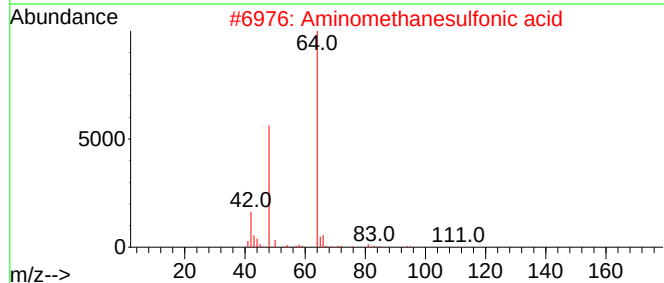
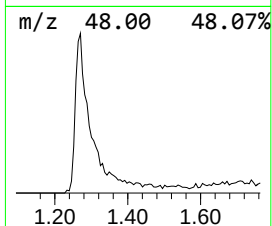
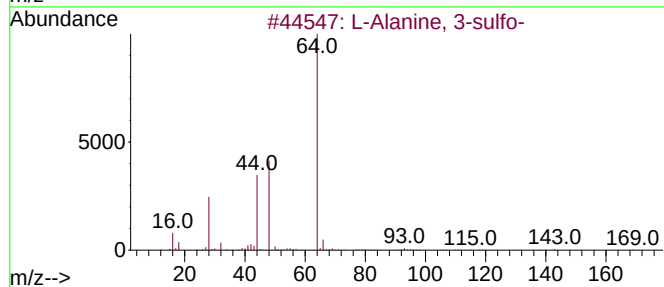
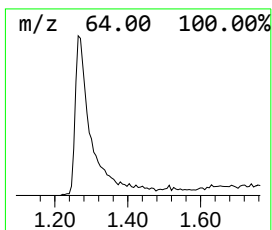
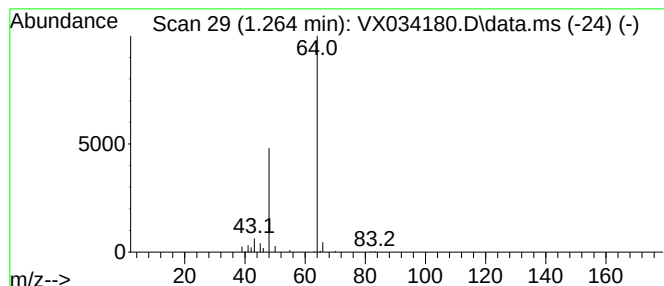
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 1 L-Alanine, 3-sulfo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	5.29 ug/l	112306	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	64
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			Sulfur dioxide	64	O2S	007446-09-5	9
4			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
L-Alanine, 3-su...	1.264	5.3	ug/l	112306	1	5.556	1060830	50.0