

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100722\
Data File : VN074800.D
Acq On : 07 Oct 2022 10:22
Operator : JC\MD
Sample : VN1007WBL01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VN1007WBL01

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_N\methods\82N100522W.M

Title : SW846 8260

Signal : TIC: VN074800.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	39	44	53	rVB2	140814	288504	8.90%	2.071%
2	2.836	126	133	148	rVB3	196117	810360	24.99%	5.816%
3	7.447	911	917	926	rVB2	18958	51359	1.58%	0.369%
4	8.177	1031	1041	1046	rBV2	414826	1007648	31.07%	7.232%
5	8.236	1046	1051	1061	rVB2	406338	907788	28.00%	6.515%
6	8.588	1098	1111	1125	rBV2	503730	1180001	36.39%	8.469%
7	9.106	1191	1199	1208	rBV	614995	1289812	39.78%	9.257%
8	10.571	1438	1448	1461	rBV	1748192	3242638	100.00%	23.272%
9	11.871	1659	1669	1678	rBV	972144	1787036	55.11%	12.826%
10	12.853	1827	1836	1843	rBV	960363	1644721	50.72%	11.804%
11	13.794	1989	1996	2004	rBV	1014923	1723593	53.15%	12.370%

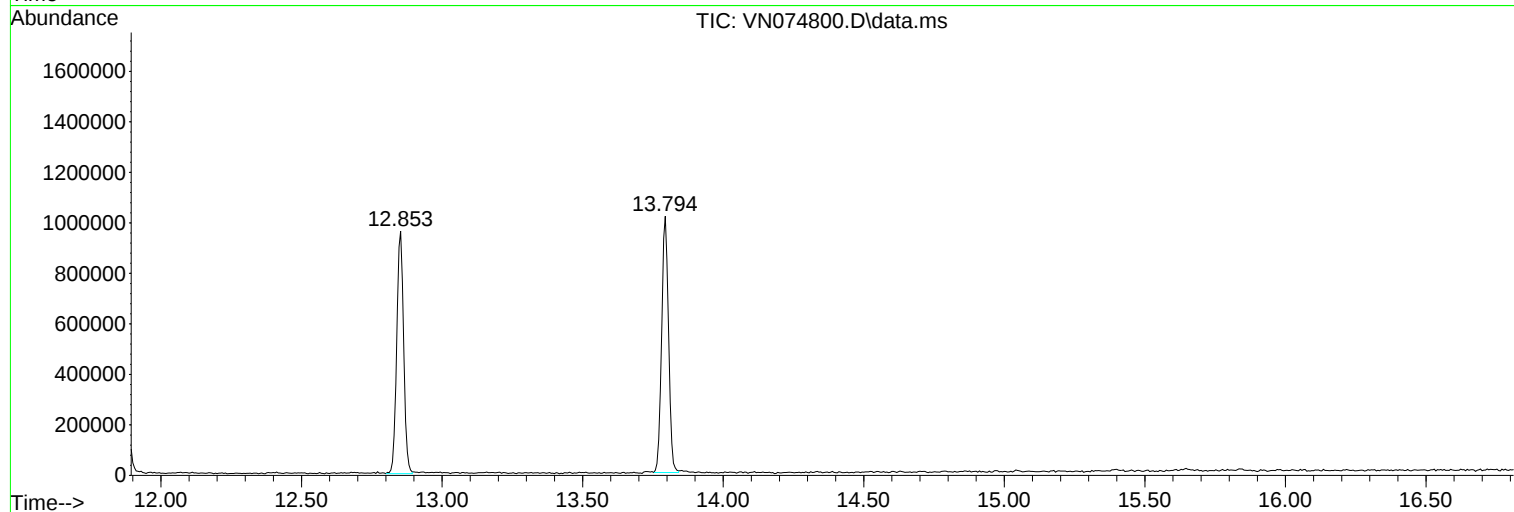
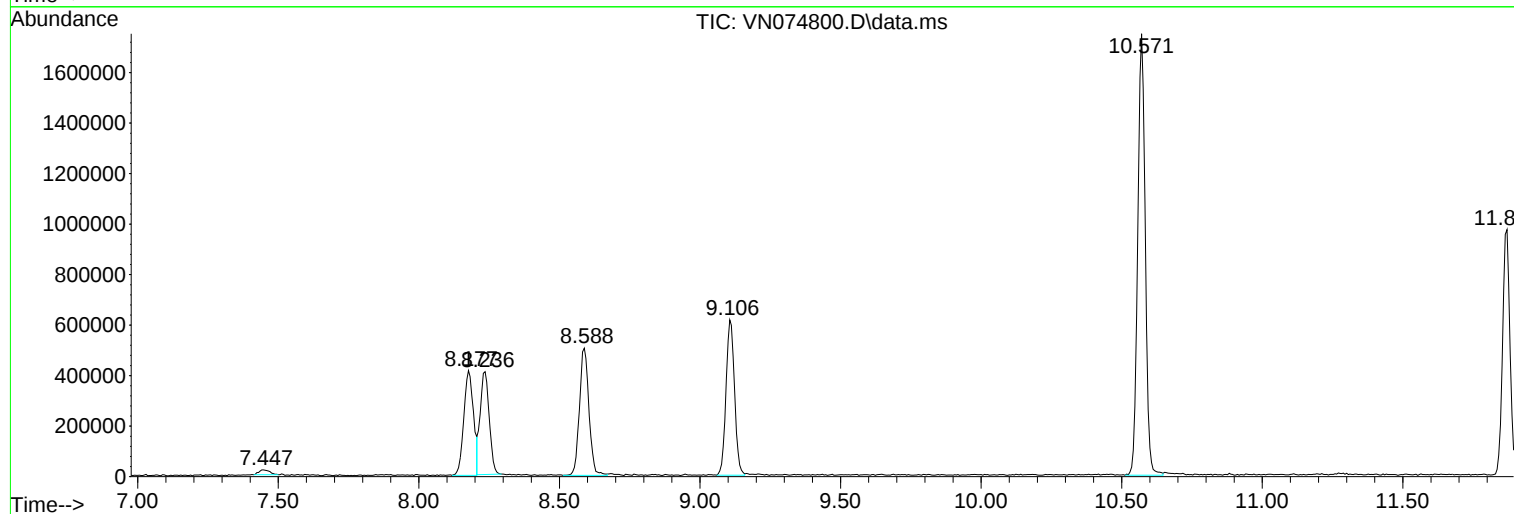
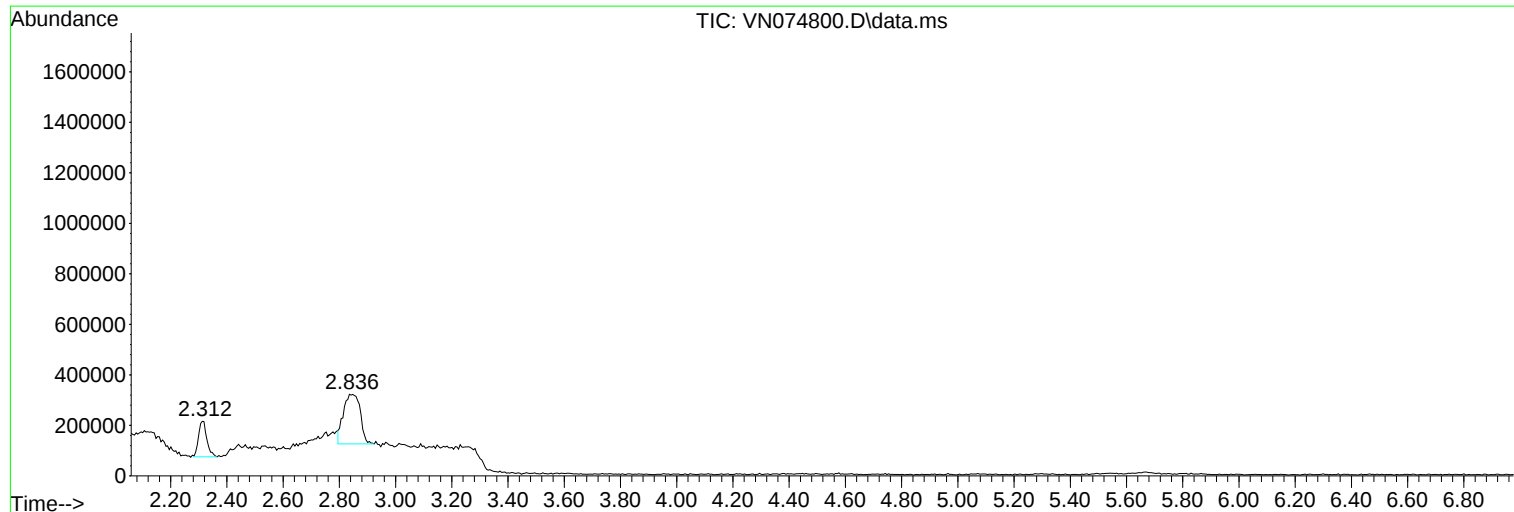
Sum of corrected areas: 13933460

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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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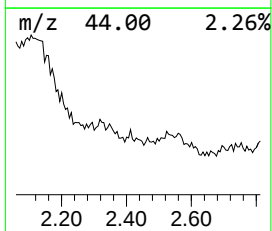
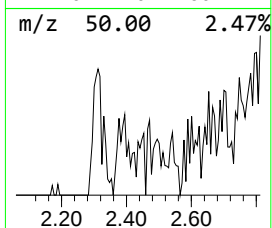
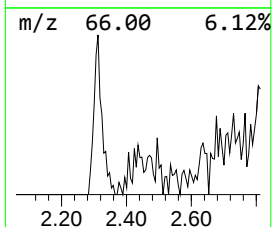
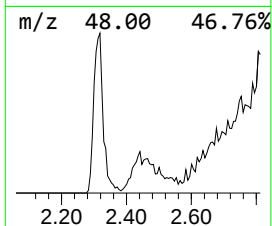
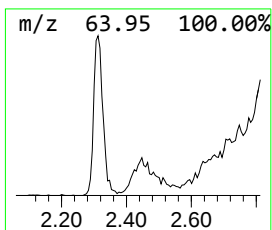
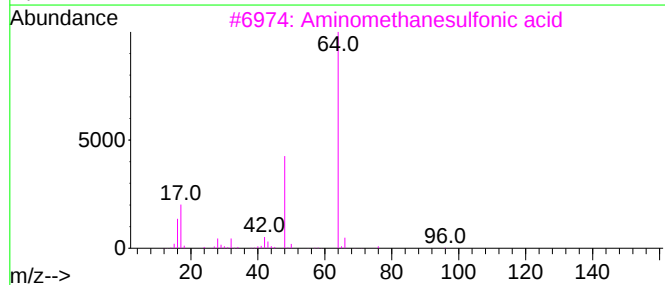
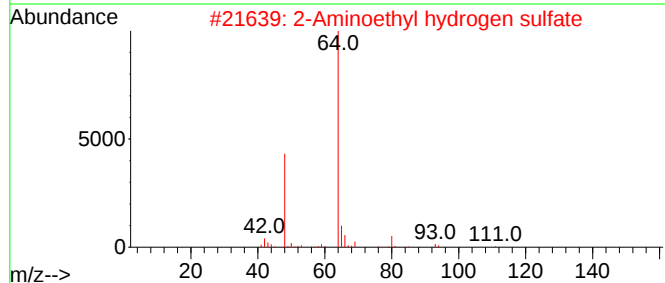
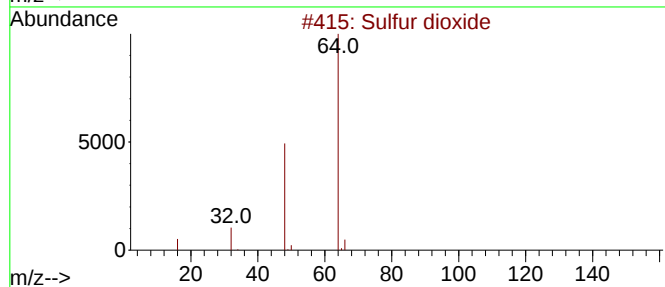
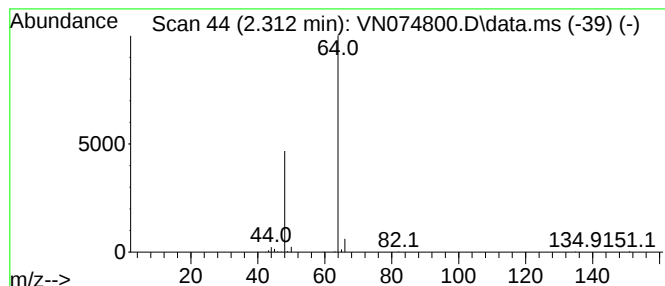
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
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Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.312	15.89 ug/l	288504	Pentafluorobenzene	8.236

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			2-Aminoethyl hydrogen sulfate	141	C2H7N04S	000926-39-6	83
3			Aminomethanesulfonic acid	111	CH5N03S	013881-91-9	74
4			1,1,1,2,2,3,3,4,4,5,5-Undecafluoro...	602	C10F22O2S	1000486-78-5	64
5			2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	64



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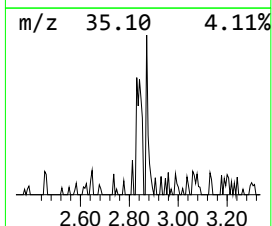
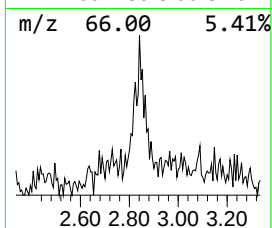
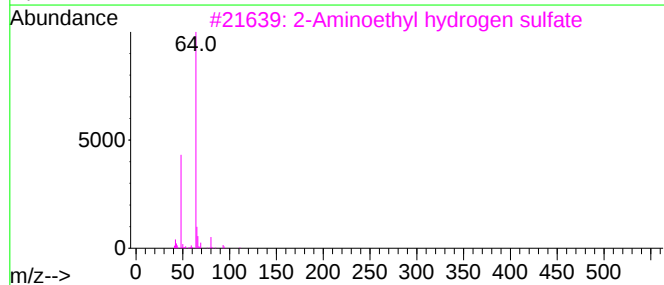
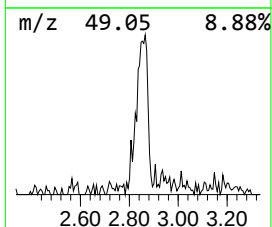
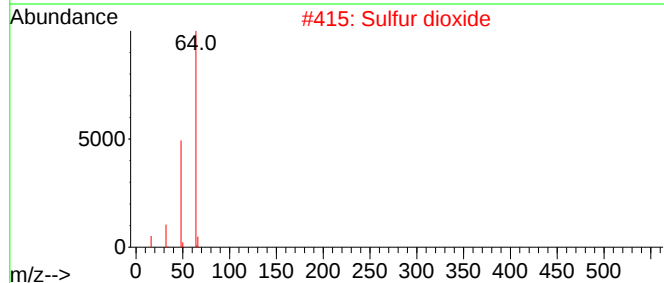
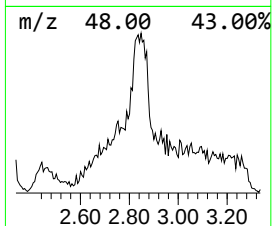
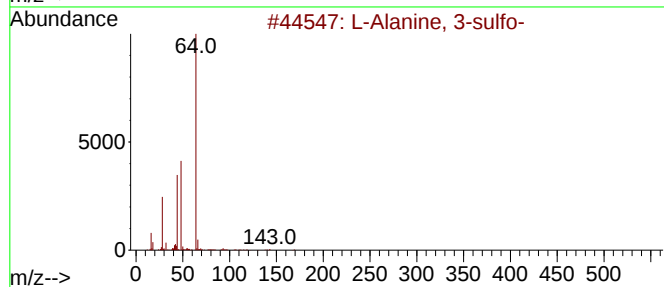
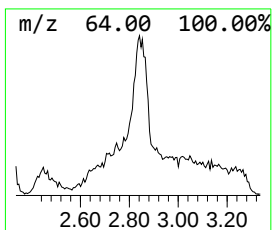
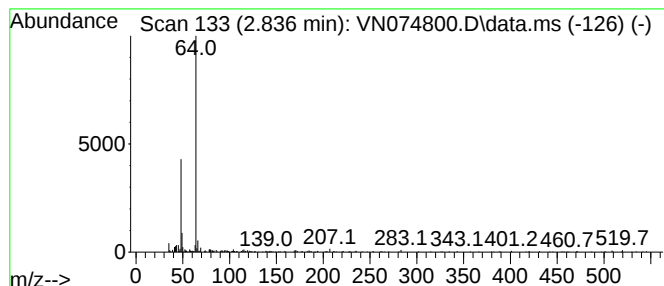
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Peak Number 2 L-Alanine, 3-sulfo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.836	44.63 ug/l	810360	Pentafluorobenzene	8.236

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	90
2			Sulfur dioxide	64	O2S	007446-09-5	90
3			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	83
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
5			N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.312	15.9	ug/l	288504	1	8.236	907788	50.0
L-Alanine, 3-su...	2.836	44.6	ug/l	810360	1	8.236	907788	50.0