

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100722\
Data File : VN074804.D
Acq On : 07 Oct 2022 12:18
Operator : JC\MD
Sample : N4966-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
257248-5

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: VN074804.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	52	rBV	380710	692989	23.69%	5.213%
2	2.830	128	132	152	rVB3	210106	816759	27.92%	6.144%
3	4.742	450	457	458	rBV3	20057	29649	1.01%	0.223%
4	4.753	458	459	469	rVB3	27034	49158	1.68%	0.370%
5	7.453	910	918	931	rVB	48217	133344	4.56%	1.003%
6	8.177	1031	1041	1046	rBV2	369918	911482	31.16%	6.856%
7	8.235	1046	1051	1061	rVB	371978	813378	27.80%	6.118%
8	8.588	1102	1111	1121	rBV	493204	1075591	36.77%	8.091%
9	9.106	1191	1199	1207	rBV	544420	1153194	39.42%	8.675%
10	10.571	1437	1448	1457	rBV	1551098	2925320	100.00%	22.005%
11	11.871	1660	1669	1680	rBV	859523	1588959	54.32%	11.953%
12	12.853	1826	1836	1849	rBV	870242	1521936	52.03%	11.448%
13	13.794	1988	1996	2008	rBV	892690	1582174	54.09%	11.901%

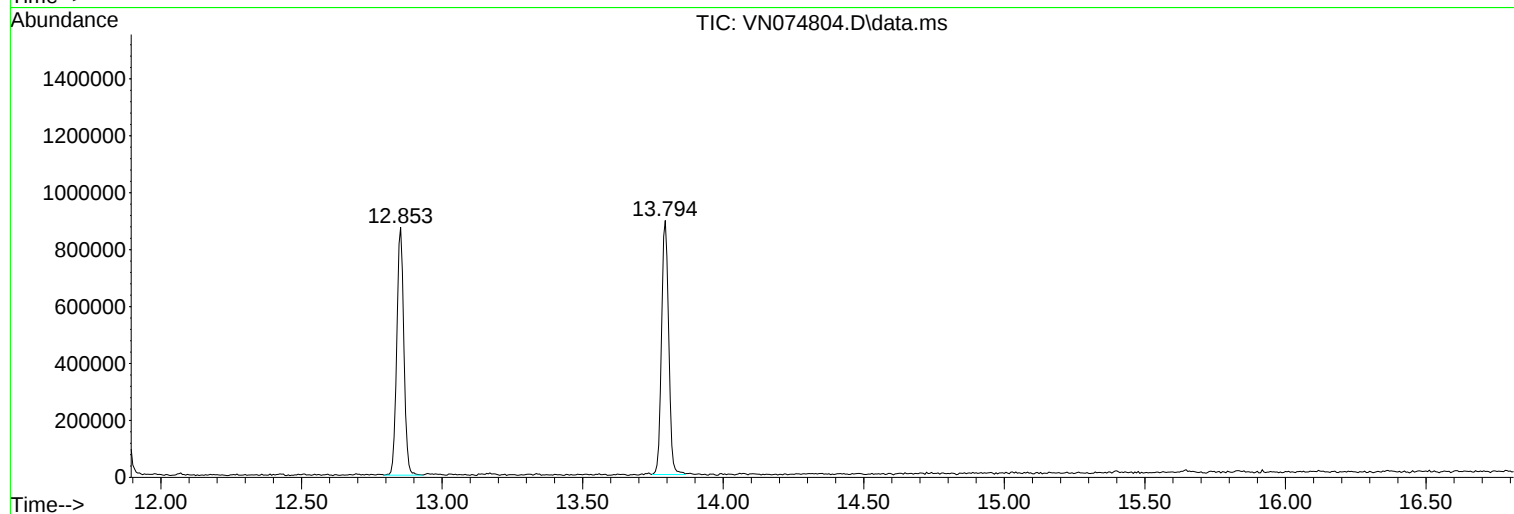
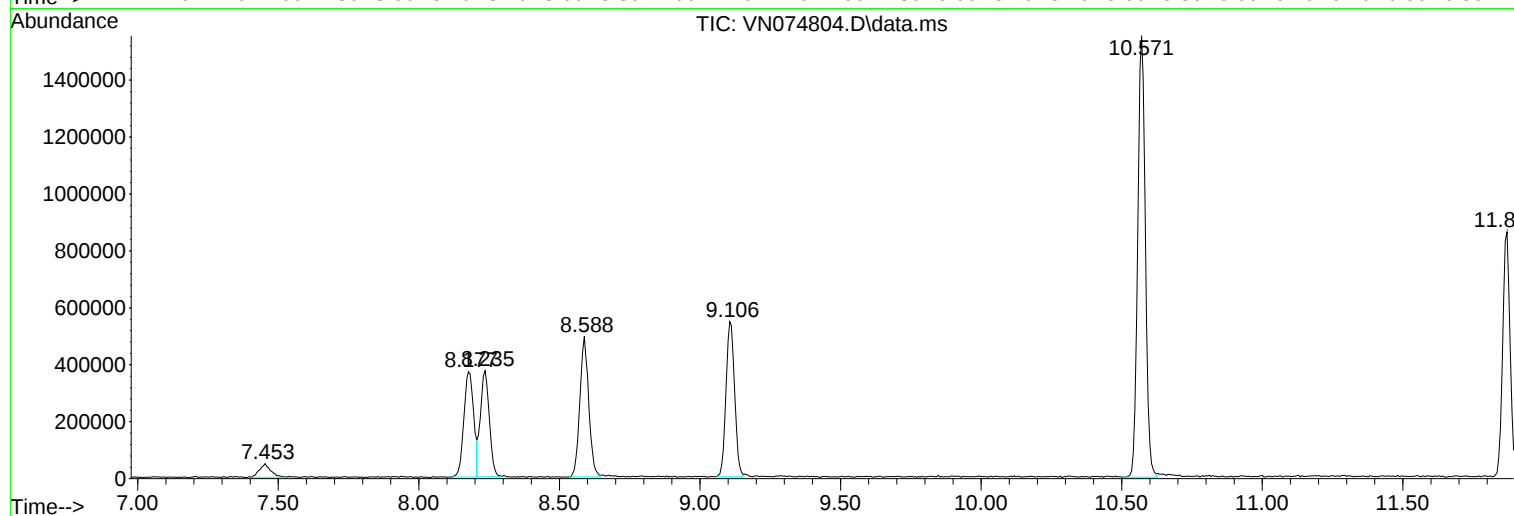
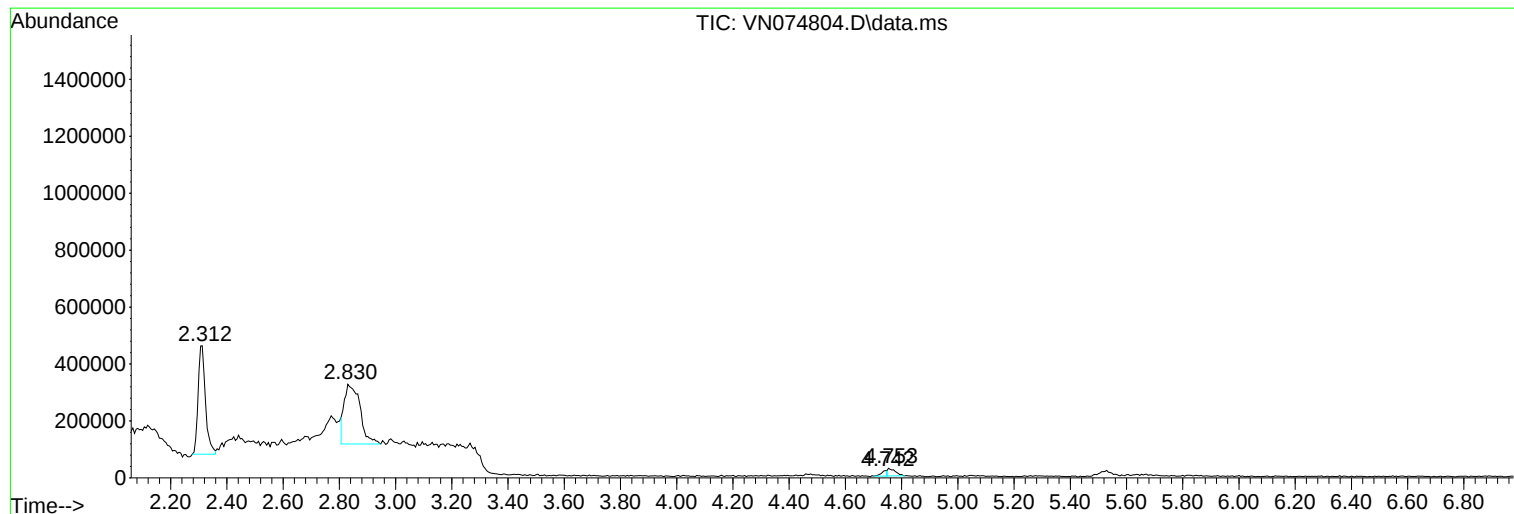
Sum of corrected areas: 13293933

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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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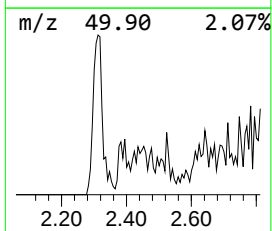
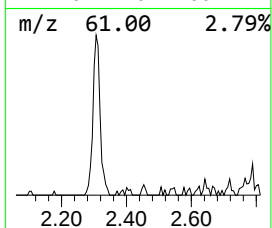
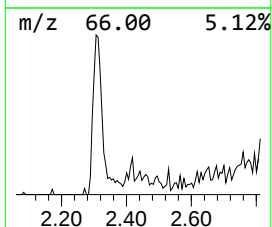
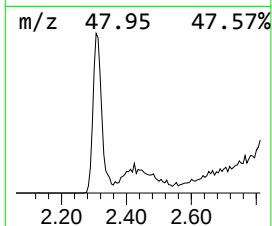
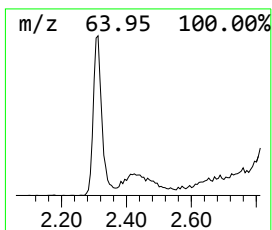
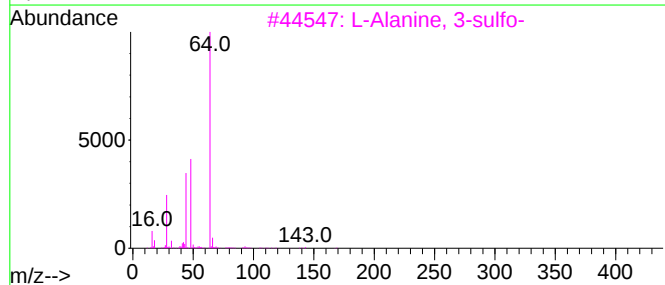
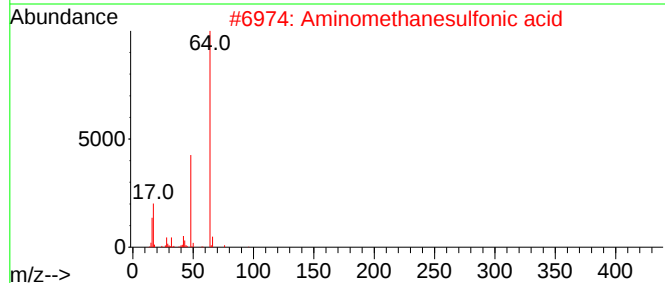
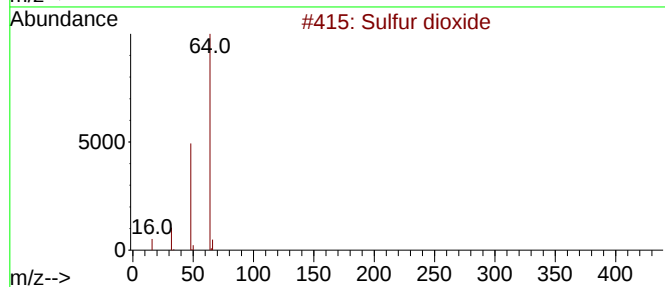
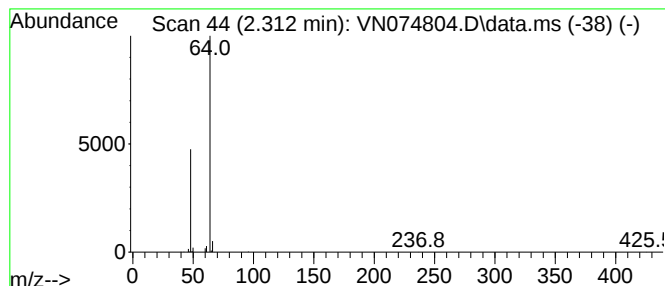
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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.
2.312	42.60 ug/l	692989	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	7
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7



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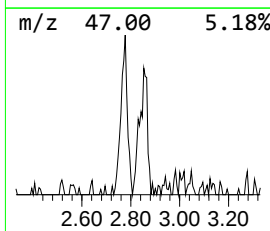
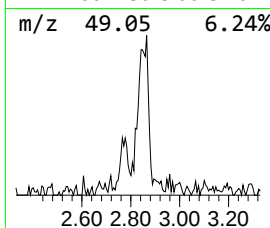
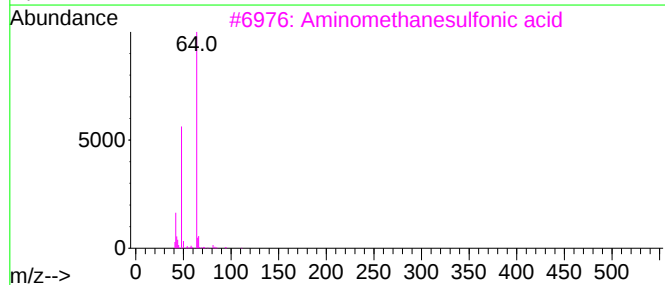
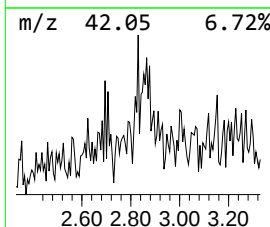
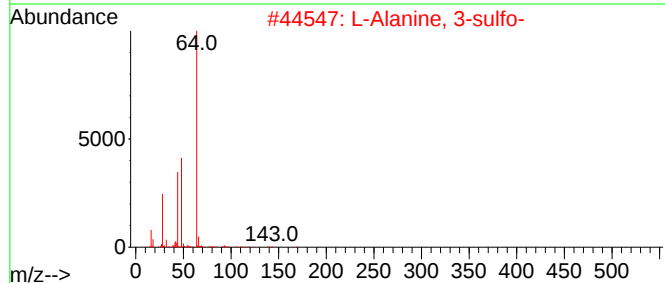
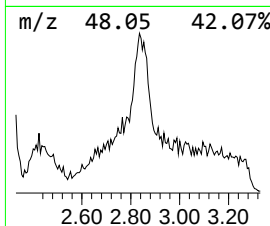
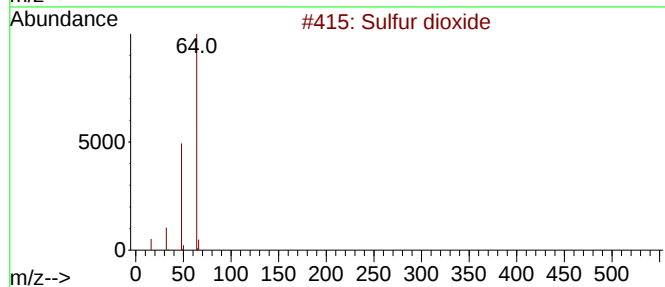
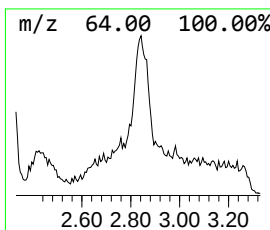
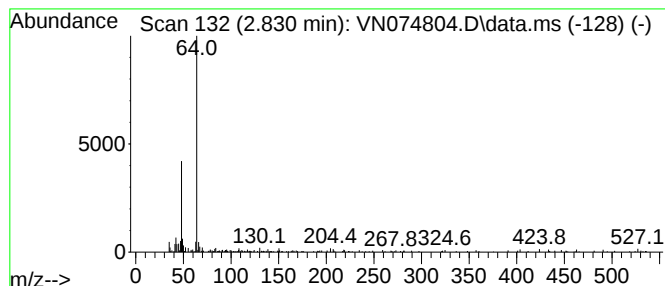
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Peak Number 2 L-Alanine, 3-sulfo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.830	50.21 ug/l	816759	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	83
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
4			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
5			Thiosulfuric acid S-[2-[[5-[O-to...	347	C15H25NO4S2	038920-47-7	64



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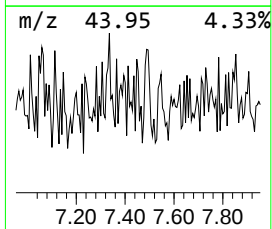
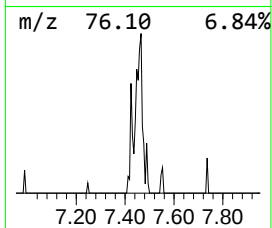
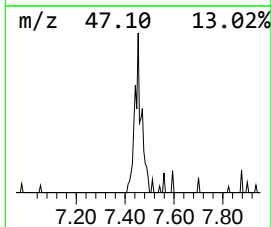
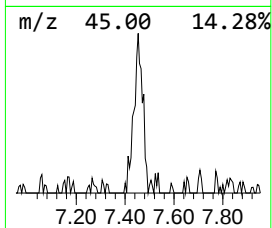
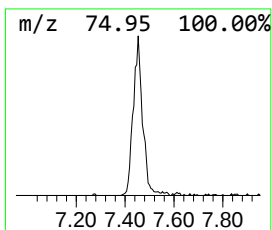
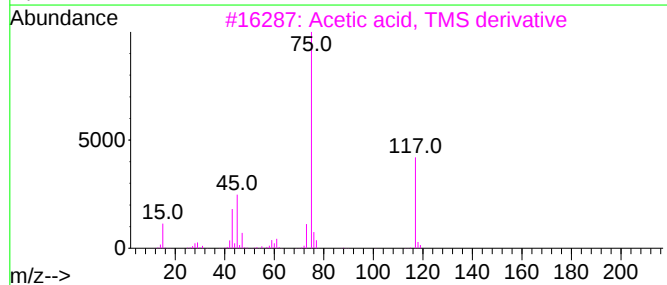
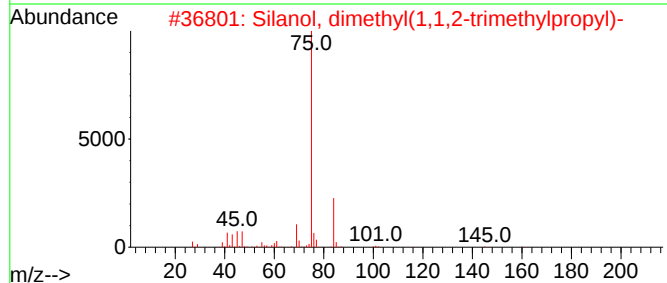
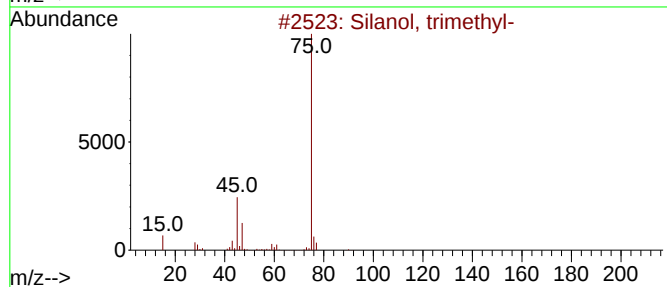
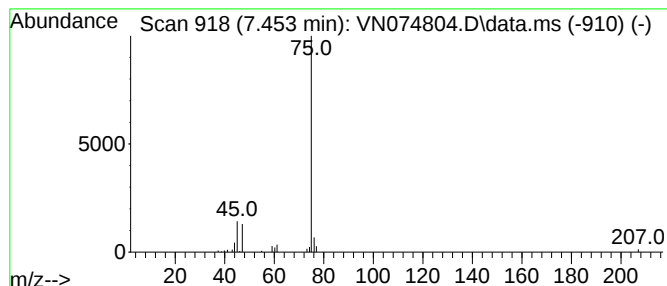
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Peak Number 3 Silanol, trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.453	8.20 ug/l	133344	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	83
2			Silanol, dimethyl(1,1,2-trimethy...	160	C8H20OSi	055644-10-5	78
3			Acetic acid, TMS derivative	132	C5H12O2Si	002754-27-0	78
4			tert-Butyldimethylsilyl nitrite	161	C6H15N02Si	1000366-61-8	43
5			Propanoic acid, TMS derivative	146	C6H14O2Si	016844-98-7	43



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.312	42.6	ug/l	692989	1	8.235	813378	50.0
L-Alanine, 3-su...	2.830	50.2	ug/l	816759	1	8.235	813378	50.0
Silanol, trimet...	7.453	8.2	ug/l	133344	1	8.235	813378	50.0