

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
 Data File : VN074593.D
 Acq On : 19 Sep 2022 18:06
 Operator : JC\MD
 Sample : N4686-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 5486-1

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_N\methods\82N091522W.M
 Title : SW846 8260

Signal : TIC: VN074593.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	47	53	61	rBV	159284	323011	20.63%	3.491%
2	2.458	91	97	98	rBV4	19586	31796	2.03%	0.344%
3	2.634	121	127	131	rBV3	43182	93965	6.00%	1.015%
4	2.699	133	138	143	rVV6	33032	90335	5.77%	0.976%
5	3.269	234	235	244	rVB5	28397	53166	3.40%	0.575%
6	4.510	441	446	457	rVB5	8257	23727	1.52%	0.256%
7	7.240	902	910	917	rBV2	7851	22743	1.45%	0.246%
8	7.951	1020	1031	1036	rBV2	217569	521214	33.29%	5.632%
9	8.016	1036	1042	1055	rVB	324236	763572	48.78%	8.251%
10	8.369	1092	1102	1114	rBV	255470	574576	36.70%	6.209%
11	8.904	1184	1193	1202	rBV2	539152	1112091	71.04%	12.018%
12	10.381	1434	1444	1460	rBV	855517	1565467	100.00%	16.917%
13	11.686	1654	1666	1677	rBV	893832	1529817	97.72%	16.532%
14	12.675	1825	1834	1846	rVB	715766	1177582	75.22%	12.725%
15	13.616	1987	1994	2001	rBV	852665	1370850	87.57%	14.814%

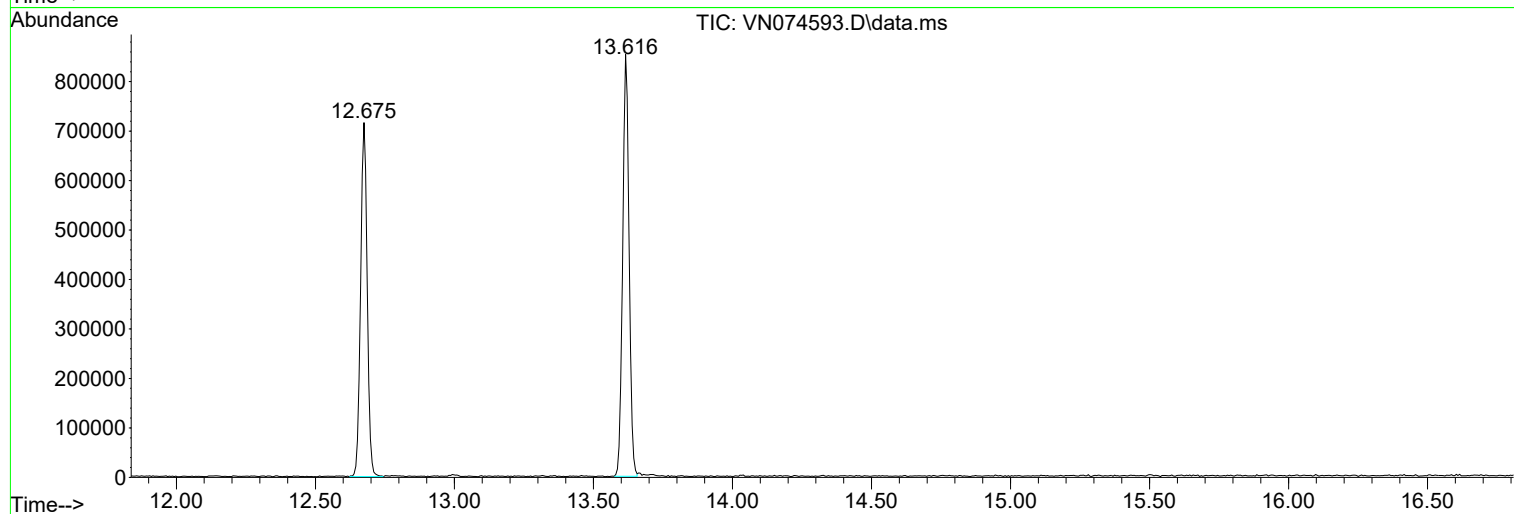
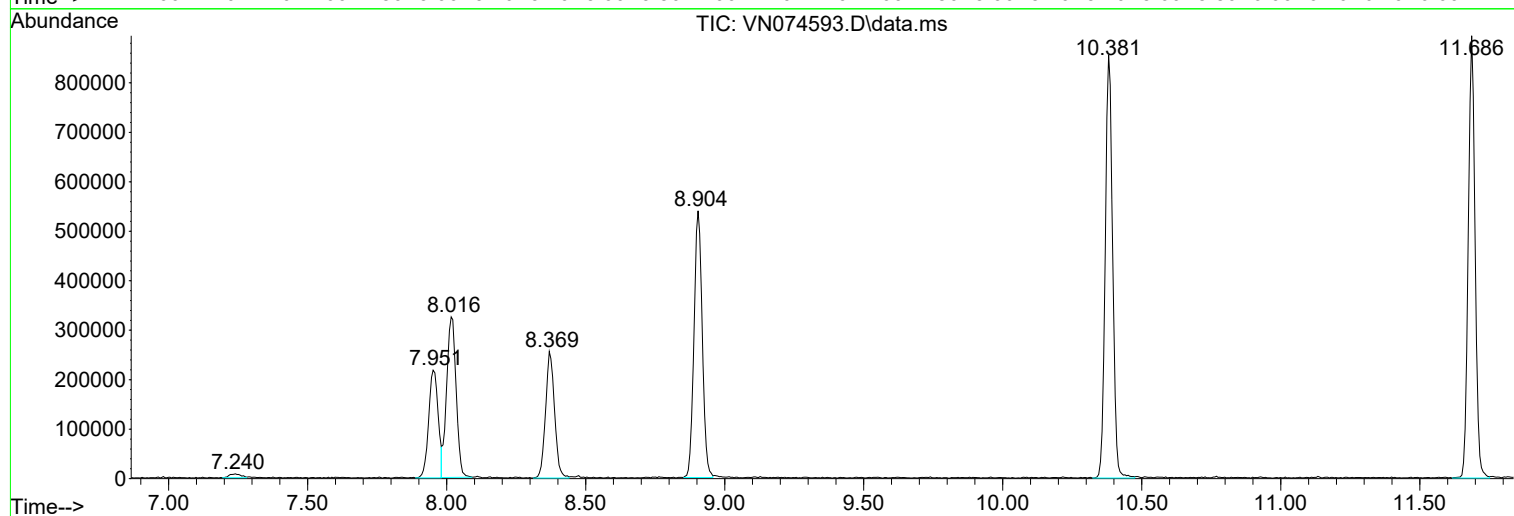
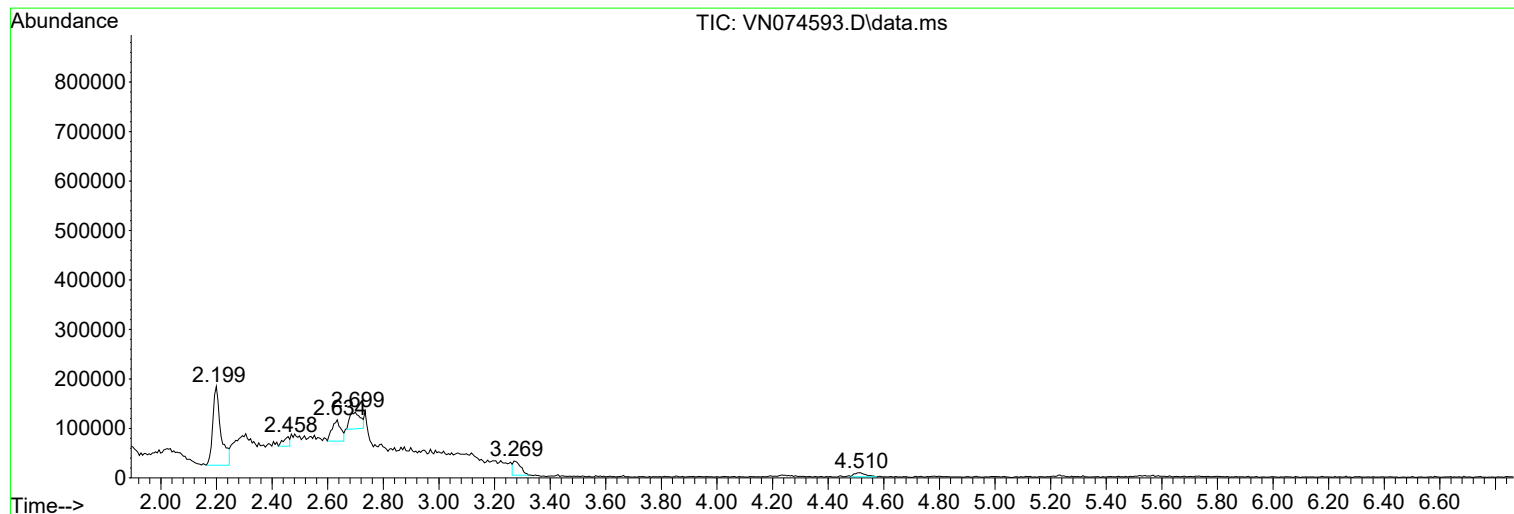
Sum of corrected areas: 9253912

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



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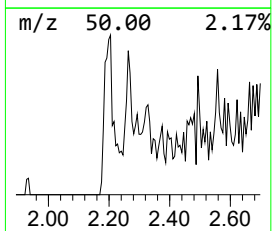
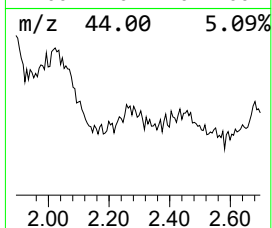
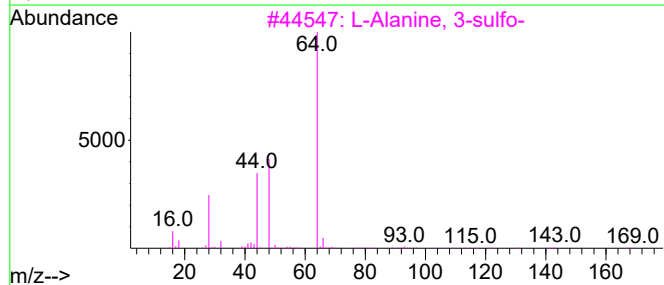
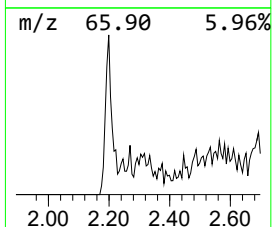
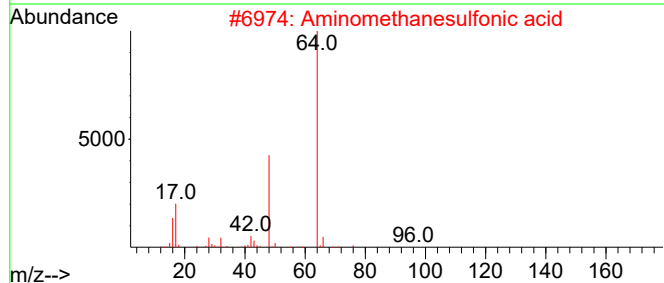
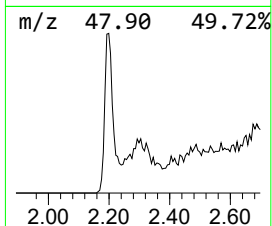
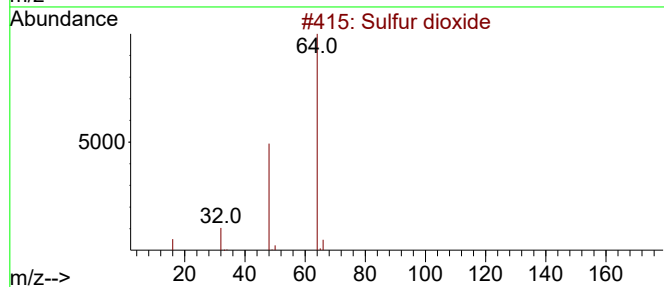
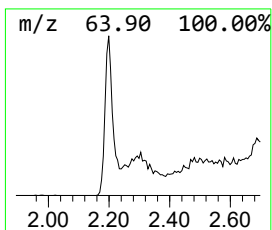
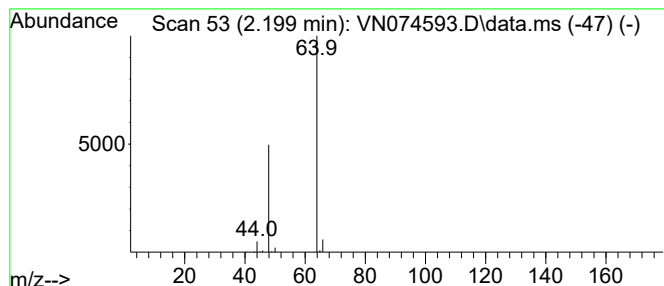
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	21.15 ug/l	323011	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
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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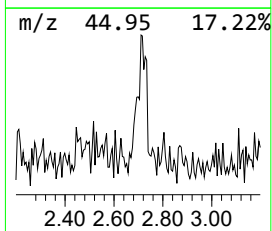
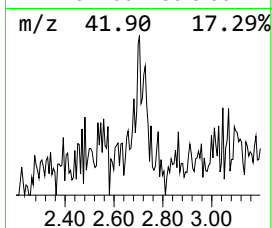
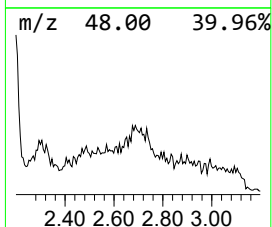
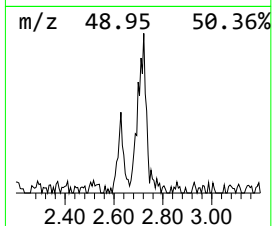
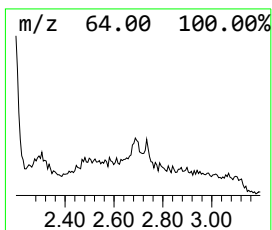
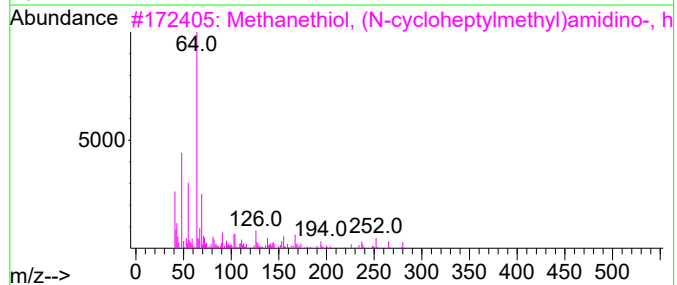
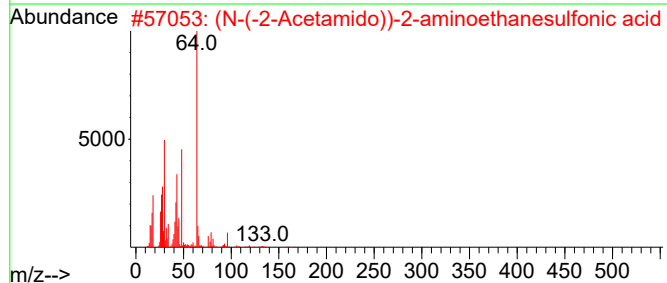
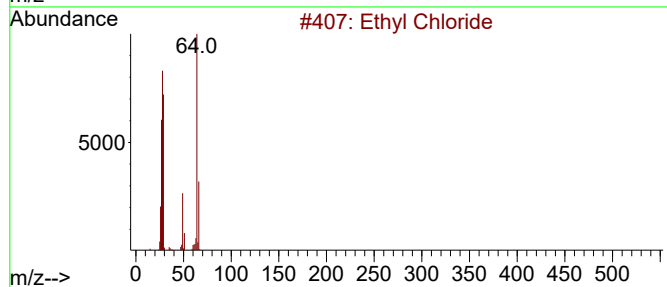
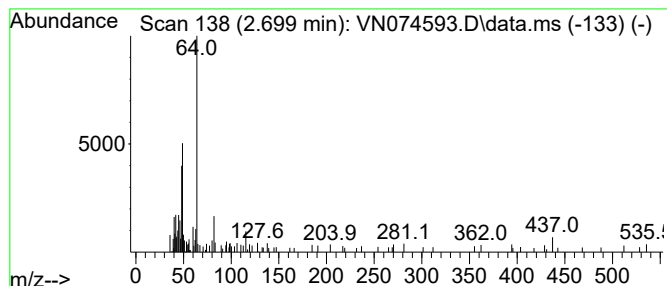
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Peak Number 3 unknown2.699 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.699	5.92 ug/l	90335	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Chloride	64	C2H5Cl	000075-00-3	72
2			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	40
3			Methanethiol, (N-cycloheptylmeth...	280	C10H20N2O3S2	040283-61-2	40
4			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	40
5			Thiosulfuric acid, S-[2-(2-hydro...	289	C11H15N2O4S2	062209-43-2	33



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	21.1	ug/l	323011	1	8.016	763572	50.0
unknown2.699	2.699	5.9	ug/l	90335	1	8.016	763572	50.0