

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074547.D
 Acq On : 17 Sep 2022 06:58
 Operator : JC\MD
 Sample : N4549-19
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 53 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-63

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: VN074547.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	60	rBV	291818	525524	27.91%	4.718%
2	2.687	132	136	142	rBV3	46679	105952	5.63%	0.951%
3	5.522	608	618	620	rBV2	28104	57225	3.04%	0.514%
4	7.228	901	908	917	rBV2	12978	36924	1.96%	0.331%
5	7.951	1021	1031	1036	rBV	266250	618244	32.84%	5.550%
6	8.016	1036	1042	1052	rVB	400313	896091	47.59%	8.045%
7	8.369	1092	1102	1112	rBV2	294734	678957	36.06%	6.096%
8	8.904	1185	1193	1203	rBV	661111	1342591	71.31%	12.053%
9	9.945	1359	1370	1378	rVB5	16271	43225	2.30%	0.388%
10	10.380	1436	1444	1452	rBV	1049819	1882759	100.00%	16.903%
11	10.580	1473	1478	1485	rVB6	13831	24744	1.31%	0.222%
12	10.663	1485	1492	1497	rBV3	15771	26407	1.40%	0.237%
13	11.686	1657	1666	1675	rBV	1051848	1820586	96.70%	16.345%
14	12.674	1823	1834	1844	rBV	842747	1405749	74.66%	12.620%
15	13.616	1987	1994	2008	rBV	1036613	1673639	88.89%	15.026%

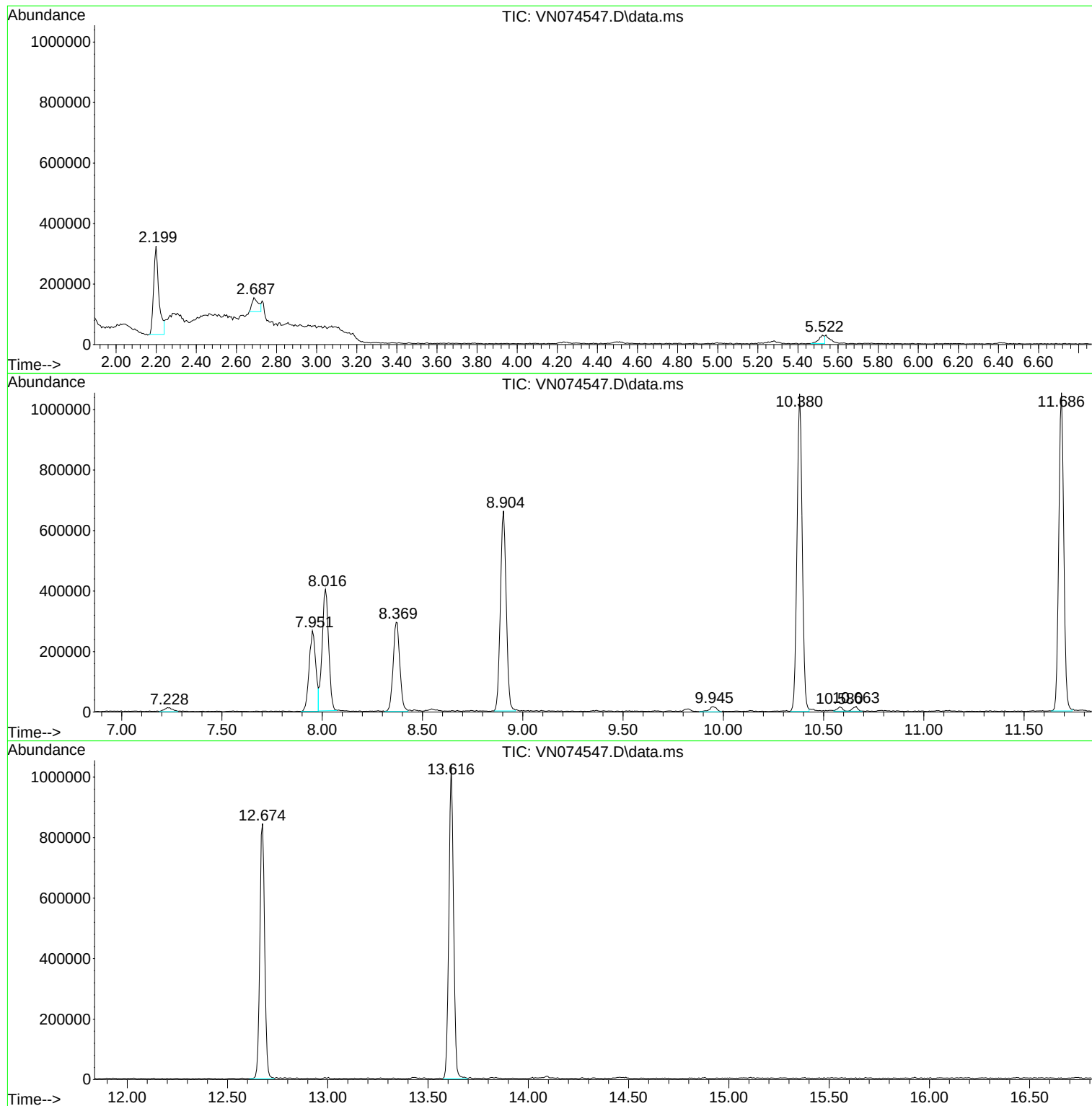
Sum of corrected areas: 11138617

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Quant Title : SW846 8260

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



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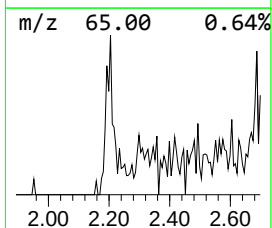
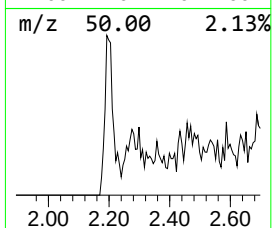
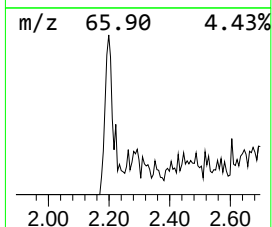
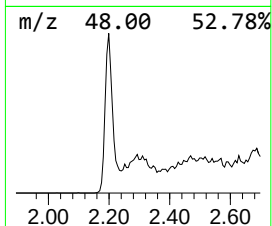
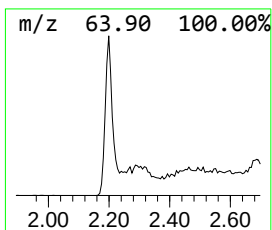
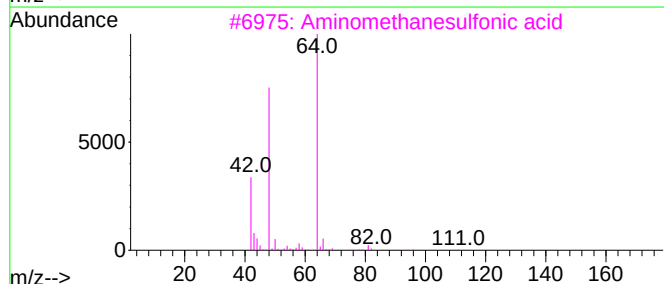
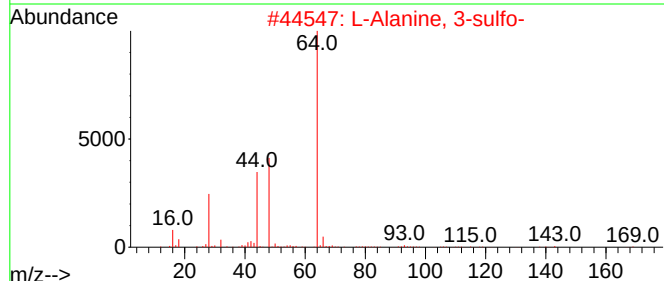
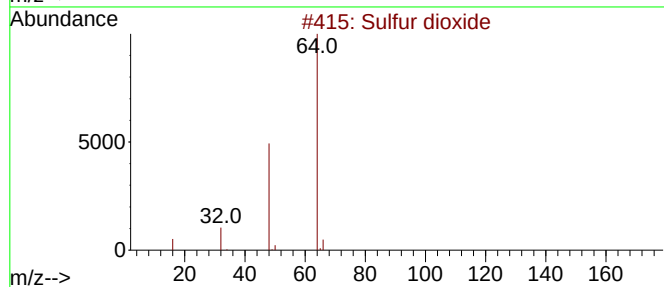
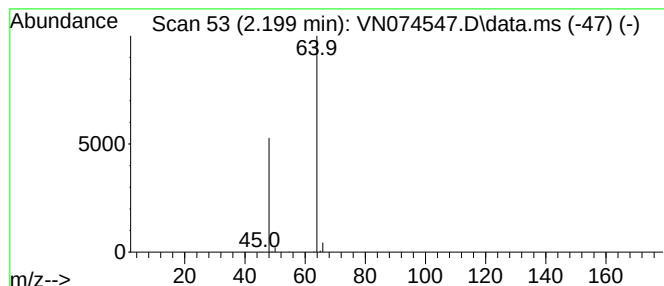
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Quant Title : SW846 8260

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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	29.32 ug/l	525524	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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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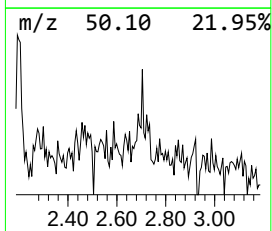
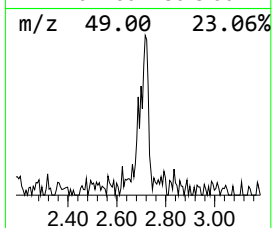
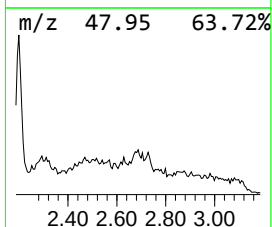
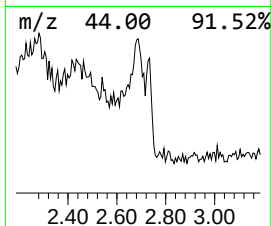
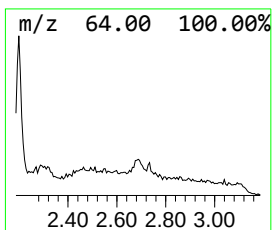
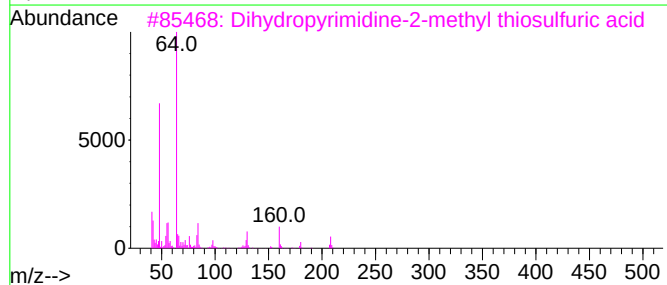
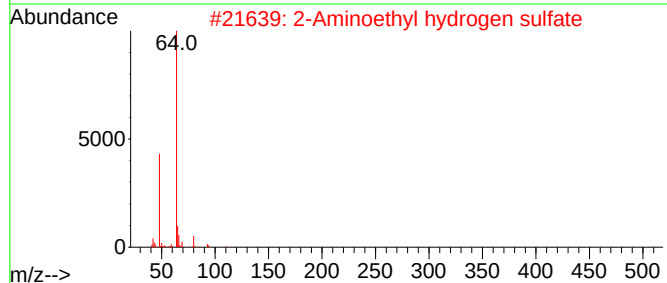
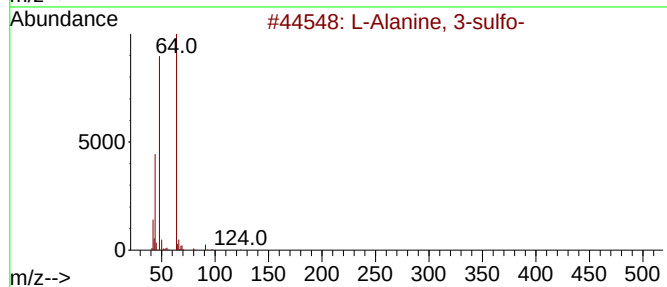
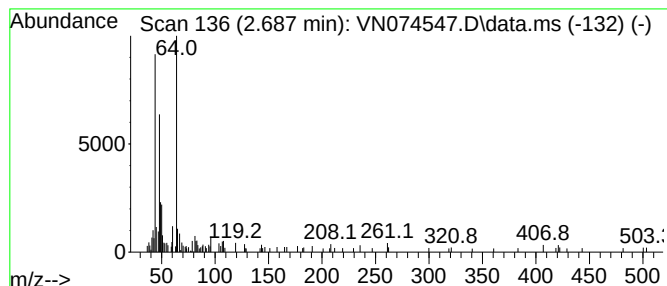
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Peak Number 2 unknown2.687 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.687	5.91 ug/l	105952	Pentafluorobenzene	8.016	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	42
2	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	40
3	Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	40
4	S-2-[2-Succinimidoethylamino]eth...	282	C8H14N2O5S2	031701-74-3	39
5	N,N'-Nonamethylenebis[-S-3-amino...	466	C15H34N2O6S4	035871-58-0	36



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	29.3	ug/l	525524	1	8.016	896091	50.0
unknown2.687	2.687	5.9	ug/l	105952	1	8.016	896091	50.0