

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
 Data File : VN074661.D
 Acq On : 30 Sep 2022 12:20
 Operator : JC\MD
 Sample : VN0930MBL01
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 VN0930MBL01

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\82N092922W.M
 Title : SW846 8260

Signal : TIC: VN074661.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	41	46	53	rBV	159324	310160	14.75%	2.461%
2	2.252	55	62	63	rBV2	90134	170697	8.12%	1.354%
3	7.128	882	891	893	rBV2	47200	81441	3.87%	0.646%
4	7.863	1007	1016	1022	rBV2	327391	820339	39.00%	6.509%
5	7.934	1022	1028	1039	rVB	502689	1160207	55.16%	9.205%
6	8.287	1079	1088	1099	rBV	324540	739171	35.14%	5.865%
7	8.828	1170	1180	1189	rBV	792302	1583456	75.28%	12.564%
8	10.310	1424	1432	1442	rBV2	943053	1734100	82.45%	13.759%
9	11.057	1556	1559	1566	rVB7	11473	22750	1.08%	0.181%
10	11.616	1646	1654	1665	rBV	1205515	2103289	100.00%	16.688%
11	12.604	1814	1822	1834	rBV	1012415	1742634	82.85%	13.827%
12	13.551	1974	1983	1994	rVV	1219535	2097550	99.73%	16.642%
13	15.363	2287	2291	2296	rVB5	23486	37785	1.80%	0.300%

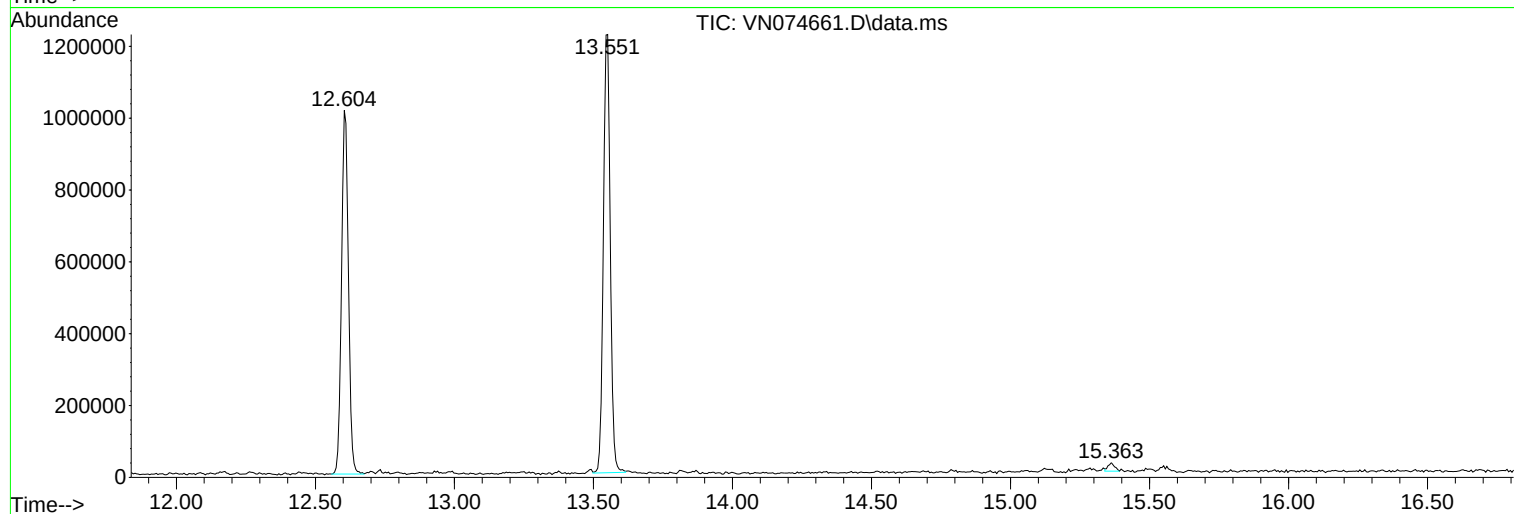
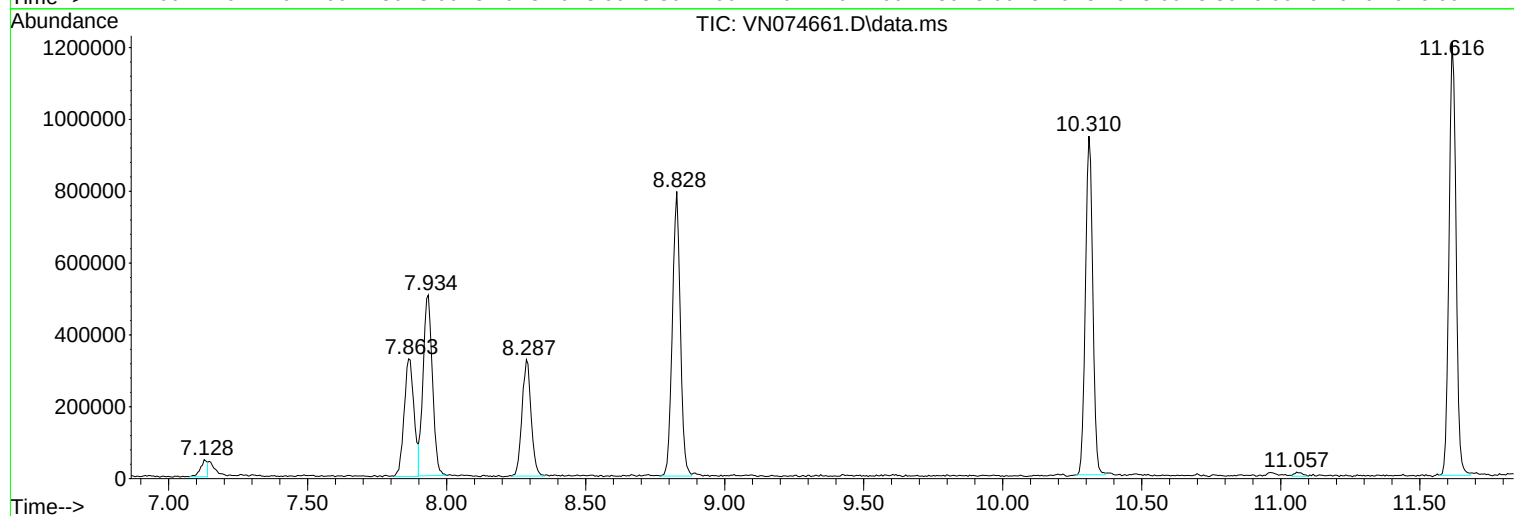
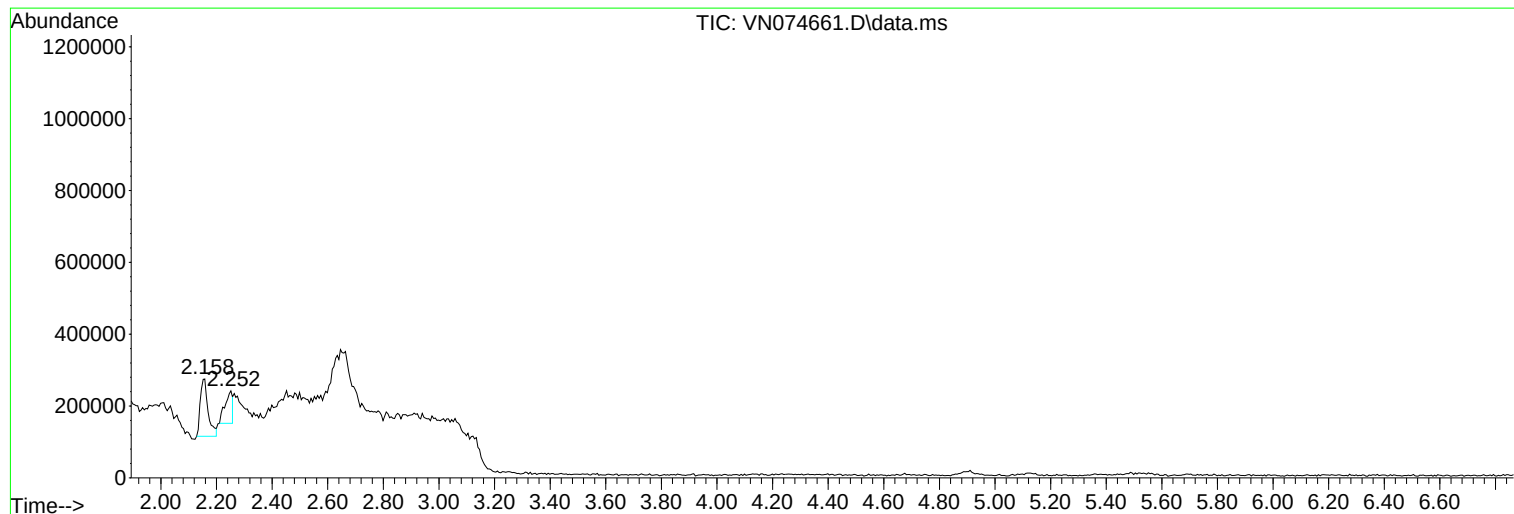
Sum of corrected areas: 12603579

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
Data File : VN074661.D
Acq On : 30 Sep 2022 12:20
Operator : JC\MD
Sample : VN0930MBL01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VN0930MBL01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
Data File : VN074661.D
Acq On : 30 Sep 2022 12:20
Operator : JC\MD
Sample : VN0930MBL01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VN0930MBL01

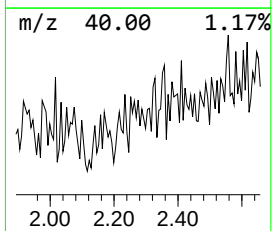
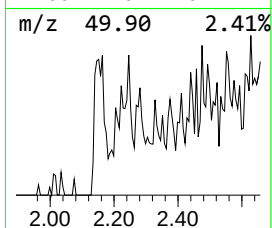
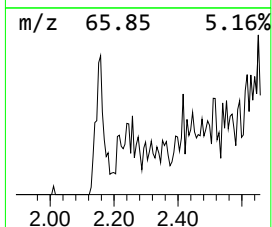
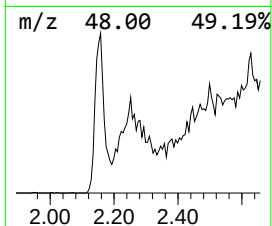
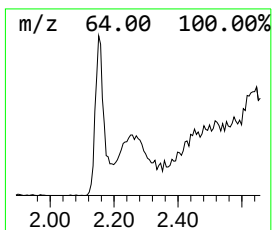
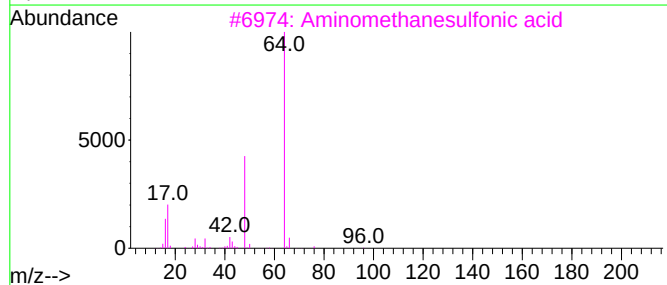
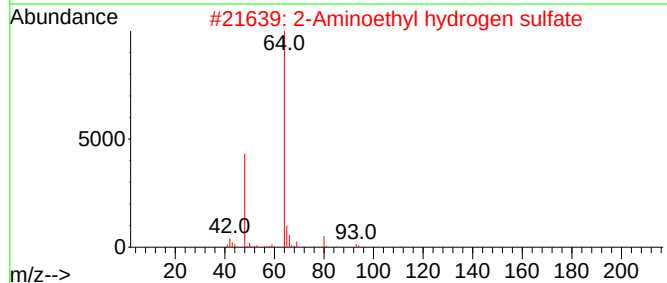
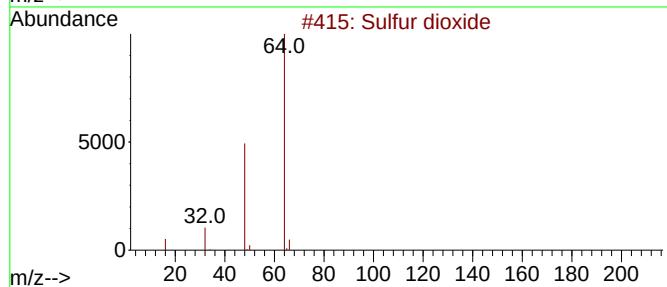
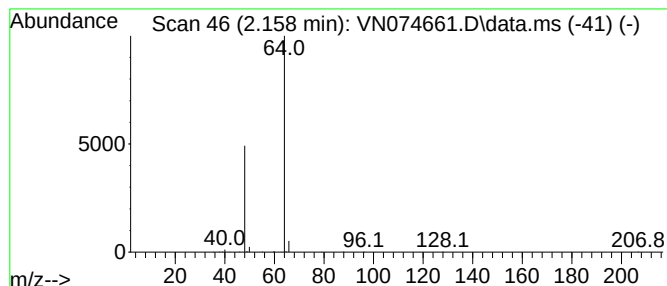
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.158	13.37 ug/l	310160	Pentafluorobenzene	7.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			2-Aminoethyl hydrogen sulfate	141	C2H7N04S	000926-39-6	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
Data File : VN074661.D
Acq On : 30 Sep 2022 12:20
Operator : JC\MD
Sample : VN0930MBL01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VN0930MBL01

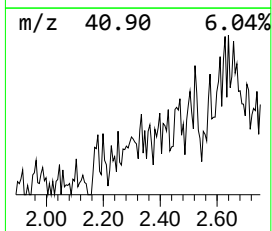
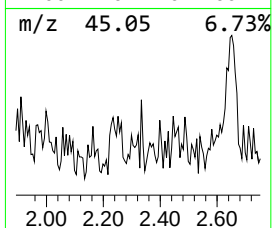
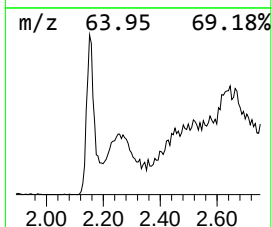
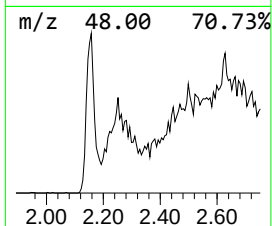
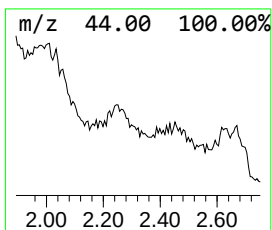
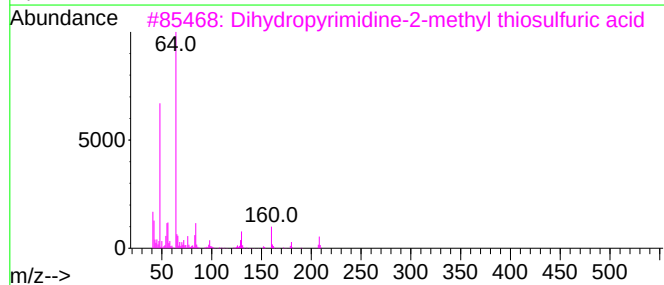
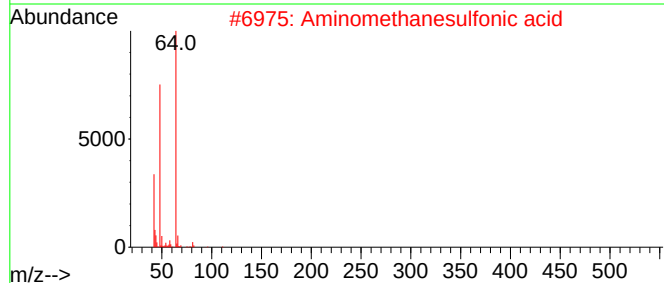
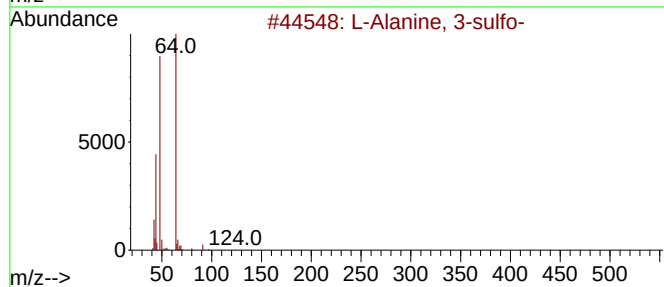
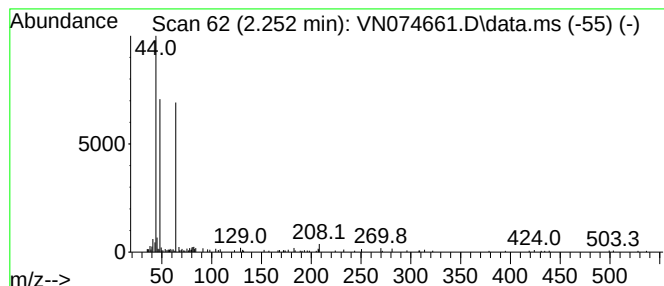
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown2.252 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	7.36 ug/l	170697	Pentafluorobenzene	7.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	39
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	33
3			Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	28
4			3,3-Dimethyl-4-methylamino-butan...	129	C7H15NO	123528-99-4	9
5			Acetic acid, [(aminocarbonyl)ami...	132	C3H4N2O4	000585-05-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
Data File : VN074661.D
Acq On : 30 Sep 2022 12:20
Operator : JC\MD
Sample : VN0930MBL01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VN0930MBL01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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	2.158	13.4	ug/l	310160	1	7.928	1160210	50.0
unknown2.252	2.252	7.4	ug/l	170697	1	7.928	1160210	50.0